Request — Jan Delaval

Access DB# 127349

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabiha Qazi Examiner #: 74141 Date: 7/14/04

Art Unit: 1616 Phone Number 30 20622 Serial Number 09/893324

Mail Box and Bldg/Room Location: 4C70, Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. ME

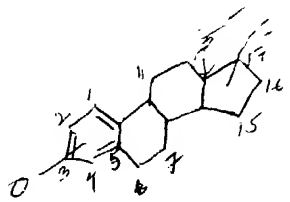
****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Alkyl ether modified Polycyclic Compds

Inventors (please provide full names): Prakash et al

Earlier applications (parent, child, divisional, or issued patent numbers) along with the appropriate serial numbers.



please search for

O—

R can be alkyl.
- St. chain, cyclic, unsaturated, saturated

Please see attached sheet

Thank you.

STAFF USE ONLY

Searcher: Jan 22504

Type of Search

Vendors and cost where applicable

Searcher Pick-up Time: 7/20

Date Completed: 7/20

Searcher Prep & Review Time:

Clerical Prep Time: 15

Online Time: 60

Dialog

Questel/Orbit

Lexis/Nexis

Sequence Systems

WWW/Internet

Other (specify)

Litigation

Fulltext

Patent Family

Other

PTO-1590 (8-01)

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FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   19 JUL 2004  HIGHEST RN 713066-32-1
DICTIONARY FILE UPDATES:  19 JUL 2004  HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l21
L9                STR
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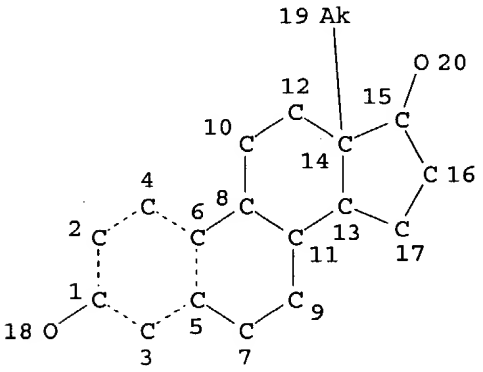


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CONNECT IS M1  RC AT  18
CONNECT IS M1  RC AT  20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
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L12             STR
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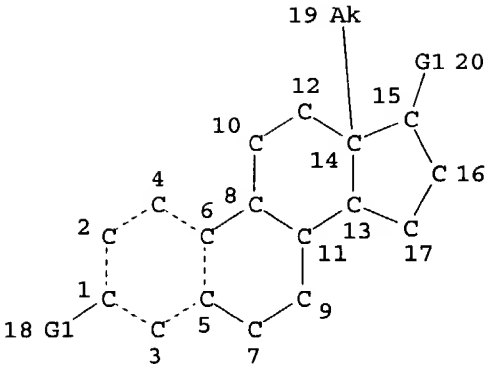

O—Ak @21 22 O—Cb @23 24 O—Ak—Cb @25 26 27

VAR G1=OH/21/23/25
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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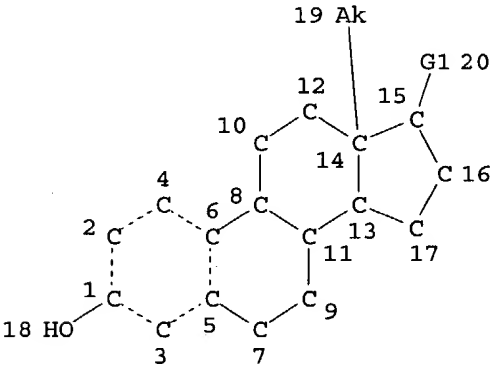

O—Ak @21 22 O—Cb @23 24 O—Ak—Cb @25 26 27

VAR G1=21/23/25
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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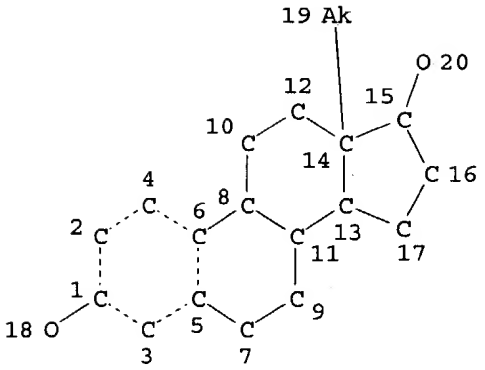

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
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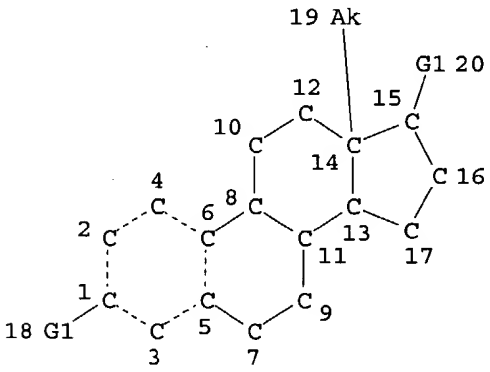

O—Ak O—Cb O—Ak—Cb
@21 22 @23 24 @25 26 27

VAR G1=OH/21/23/25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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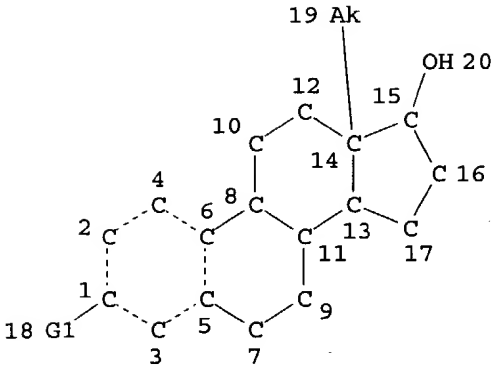
L15 119 SEA FILE=REGISTRY ABB=ON PLU=ON L14 AND NC>=2
L22 STR



O—Ak @21 22 O—Cb @23 24 O—Ak—Cb @25 26 27

VAR G1=21/23/25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L23 99 SEA FILE=REGISTRY SUB=L14 SSS FUL L22
L24 95 SEA FILE=REGISTRY ABB=ON PLU=ON L23 NOT L15
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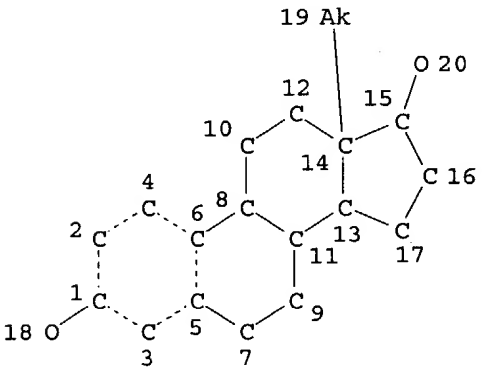
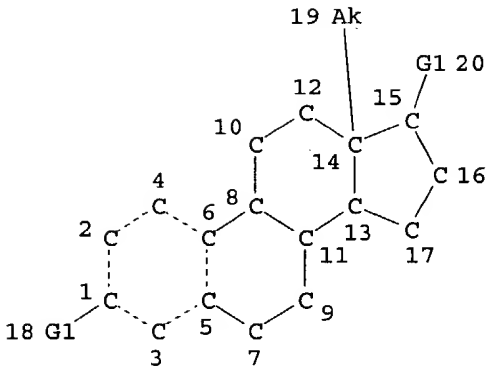
=> d sta que l32
L9 STR



NODE ATTRIBUTES:
CONNECT IS M1 RC AT 18
CONNECT IS M1 RC AT 20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L11 13381 SEA FILE=REGISTRY SSS FUL L9
L12 STR



O—Ak @21 22 O—Cb @23 24 O—Ak—Cb @25 26 27

VAR G1=OH/21/23/25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
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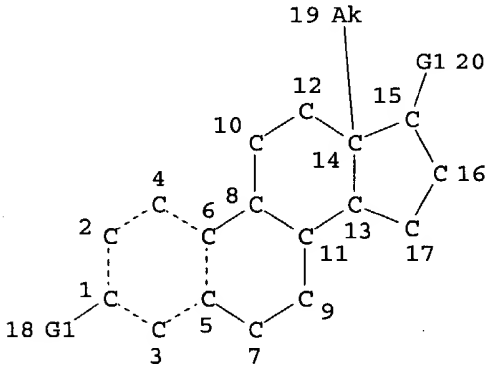

O—Ak @21 22 O—Cb @23 24 O—Ak—Cb @25 26 27

VAR G1=21/23/25
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE
L31 58 SEA FILE=REGISTRY SUB=L14 SSS FUL L30
L32 57 SEA FILE=REGISTRY ABB=ON PLU=ON L31 NOT (T OR D)/ELS

=> d his

(FILE 'HOME' ENTERED AT 10:33:36 ON 20 JUL 2004)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 10:34:03 ON 20 JUL 2004

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L1            1 S US20020035100/PN OR (US2001-893324# OR WO2001-US41170 OR US20
                E PROKAI L/AU
L2          122 S E3,E4,E7
                E SIMPKINS J/AU
L3          245 S E3,E5,E7-E9
                SEL RN L1

     FILE 'REGISTRY' ENTERED AT 10:35:20 ON 20 JUL 2004
L4           18 S E1-E18
L5           16 S L4 AND C5-C6-C6-C6/ES
L6            9 S L5 AND 4/NR
L7            7 S L5 NOT L6
L8              STR
L9              STR L8
L10          50 S L9
L11       13381 S L9 FUL
                SAV TEMP L11 QAZI893/A
L12             STR L9
L13          22 S L12 CSS SAM SUB=L11
L14         434 S L12 CSS FUL SUB=L11
                SAV L14 QAZI893A/A
L15         119 S L14 AND NC>=2
L16          13 S L15 NOT ((MXS OR PMS OR IDS)/CI OR COMPD OR WITH OR UNSPECIFI
L17           2 S L16 NOT C18H2402
L18          11 S L16 NOT L17
L19             STR L12
L20          23 S L19 FUL SUB=L14
                SAV L20 QAZI893B/A
L21          22 S L20 NOT 13C#
L22             STR L19
L23          99 S L22 FUL SUB=L14
                SAV L23 QAZI893C/A
L24          95 S L23 NOT L15
L25          87 S L24 NOT (T OR D)/ELS
L26          12 S L23 NOT L25
L27           9 S L26 AND C19H2602
L28           3 S L26 AND C19H2602 NOT (T OR D)/ELS
L29           2 S L28 NOT CYCLODEXTRIN
L30             STR L19
L31          58 S L30 FUL SUB=L14
                SAV L31 QAZI893D/A
L32          57 S L31 NOT (T OR D)/ELS
L33         169 S L5,L17,L21,L25,L29,L32
                SAV L33 QAZI893E/A
L34         168 S L33 NOT (T OR D)/ELS
L35         149 S L14 NOT L15,L34
L36          89 S L35 NOT (T OR D)/ELS
L37          46 S L36 NOT IDS/CI
L38          41 S L37 NOT (11C# OR 13C# OR 14C#)
L39          39 S L38 NOT PMS/CI

     FILE 'HCAPLUS' ENTERED AT 11:19:38 ON 20 JUL 2004
L40       52840 S L34
L41        1346 S L39
L42       53115 S L40,L41
L43          98 S L1-L3 AND L42

     FILE 'REGISTRY' ENTERED AT 11:20:19 ON 20 JUL 2004
L44           1 S 50-28-2
L45         167 S L34 NOT L44
L46          38 S L39 NOT 57-91-0

     FILE 'HCAPLUS' ENTERED AT 11:21:54 ON 20 JUL 2004
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L47          605 S L45
L48          148 S L46
L49          715 S L47,L48
L50            9 S L1-L3 AND L49
L51          706 S L49 NOT L50
L52          654 S L51 AND (PD<=20000627 OR AD<=20000627 OR PRD<=20000627)

     FILE 'REGISTRY' ENTERED AT 11:24:14 ON 20 JUL 2004
L53           33 S L45,L46 AND (C26H40O2 OR C24H36O2 OR C22H32O2)
L54            5 S L20 AND L53
L55           28 S L53 NOT L54
L56           18 S L20 NOT L54
L57           17 S L56 NOT 13C#

     FILE 'HCAPLUS' ENTERED AT 11:26:54 ON 20 JUL 2004
L58           41 S L54 OR L57
L59           33 S L58 AND L52

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:27:18 ON 20 JUL 2004
L60            5 S L54 OR L57

     FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004

=> fil uspatall
FILE 'USPATFULL' ENTERED AT 11:29:09 ON 20 JUL 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 11:29:09 ON 20 JUL 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

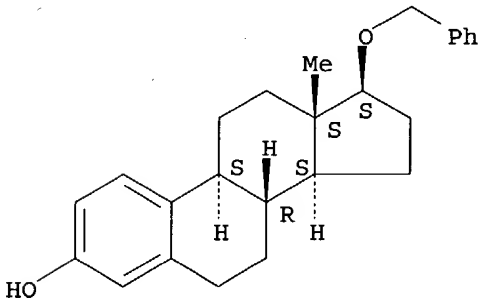
=> d l60 bib abs hitstr tot

L60  ANSWER 1 OF 5  USPATFULL on STN
AN     2002:340319  USPATFULL
TI     Extended release growth promoting two component composition
IN     Cady, Susan Mancini, Yardley, PA, United States
       Macar, Claude, Paris, FRANCE
       Gibson, John W., Springville, AL, United States
PA     Akzo Nobel N.V., Amhem, NETHERLANDS (non-U.S. corporation)
       Southern BioSystems, Birmingham, AL, United States (U.S. corporation)
PI     US 6498153          B1   20021224
AI     US 1999-273862           19990322 (9)
PRAI   FR 1998-16707       19981231
DT     Utility
FS     GRANTED
EXNAM  Primary Examiner: Badio, Barbara P.
LREP   Blackstone, William M.
CLMN   Number of Claims: 46
ECL    Exemplary Claim: 1
DRWN   0 Drawing Figure(s); 0 Drawing Page(s)
LN.CNT 776
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB     An extended release composition comprising a first composition
       comprising growth promoters and a second composition comprising growth
       promoters and a biodegradable polymer is described. A method of
       increasing weight gain in food animals utilizing the composition, a
       pharmaceutical dosage form containing the composition and a method of
       preparing the pharmaceutical dosage form are also described, as are
       pellets of the composition for implantation in food animals.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT  55561-42-7
        (pellets containing growth promoters and biodegradable polymers for
```

controlled-release implants for farm animals)
RN 55561-42-7 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

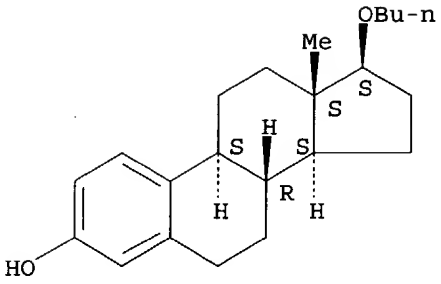
Absolute stereochemistry.



L60 ANSWER 2 OF 5 USPATFULL on STN
AN 2002:61264 USPATFULL
TI Alkyl ether modified polycyclic compounds having a terminal phenol and uses for protection of cells
IN Prokai, Laszlo, Gainesville, FL, UNITED STATES
Simpkins, James W., Fort Worth, TX, UNITED STATES
PI US 2002035100 A1 20020321
AI US 2001-893324 A1 20010627 (9)
PRAI US 2000-214077P 20000627 (60)
DT Utility
FS APPLICATION
LREP BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618
CLMN Number of Claims: 46
ECL Exemplary Claim: 1
DRWN 5 Drawing Page(s)
LN.CNT 951
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Methods and compositions are provided for achieving a cytoprotective effect by selecting a polycyclic compound with a phenol group at one end of the molecule and a carbon ring at the other such that an alkyl ether functional group in which the alkyl group has a formula C.sub.nH.sub.2n+1 (where n is at least 3 and less than 20) is positioned on the carbon ring. The compound may be used to achieve a cytoprotective effect in cells and to retard the development of a degenerative condition in a subject suffering from a disease, trauma or aging.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **319427-05-9P**
(crystal structure)
RN 319427-05-9 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17β)- (9CI) (CA INDEX NAME)

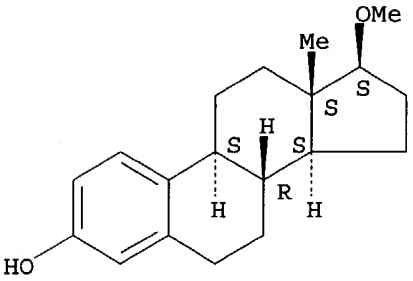
Absolute stereochemistry.



IT **4954-12-5P 319427-03-7P 319427-04-8P 319427-06-0P 319427-07-1P**
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

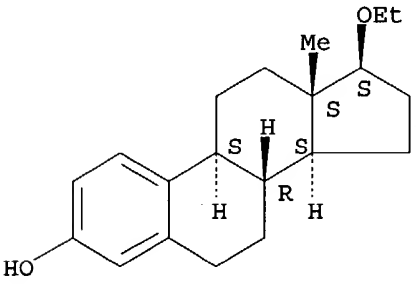
RN 4954-12-5 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



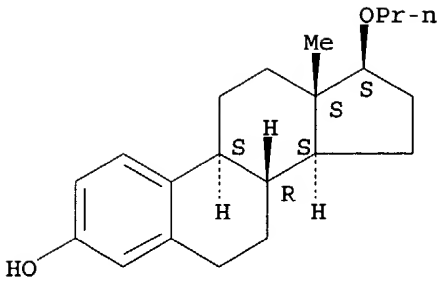
RN 319427-03-7 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



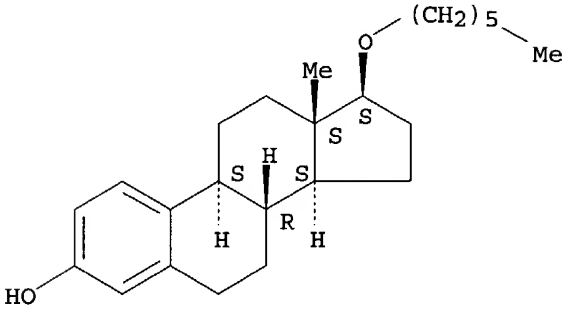
RN 319427-04-8 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



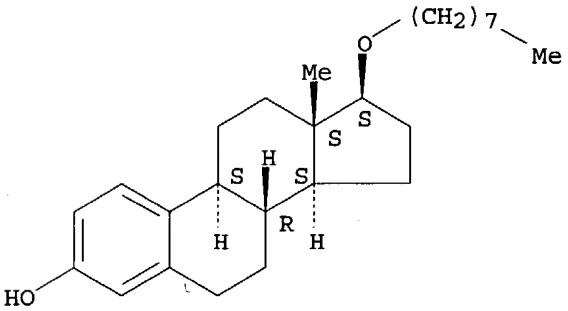
RN 319427-06-0 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-07-1 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

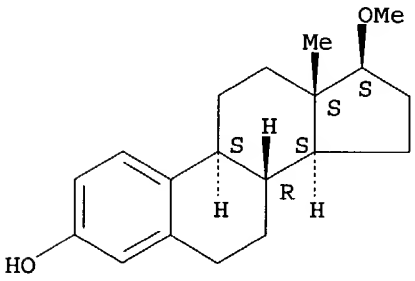


L60 ANSWER 3 OF 5 USPATFULL on STN
AN 1999:7375 USPATFULL
TI Steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5861388 19990119
AI US 1997-1601 19971231

RLI Division of Ser. No. US 1997-794229, filed on 29 Jan 1997, now patented, Pat. No. US 5763432
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Bodio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 22
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1778
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **4954-12-5**
(preparation of steroid inhibitors of estrone sulfatase)
RN 4954-12-5 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

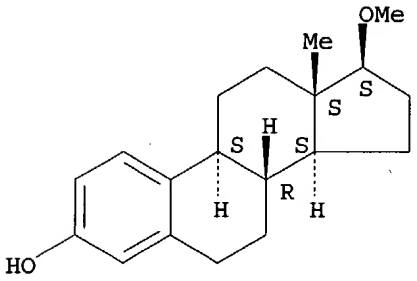


L60 ANSWER 4 OF 5 USPATFULL on STN
AN 1998:65215 USPATFULL
TI Steriod inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato, Palo Alto, CA, United States
Peters, Richard H., San Jose, CA, United States
Chao, Wan-Ru, Sunnyvale, CA, United States
Shigeno, Kazuhiko, Mountain View, CA, United States
PA SRI International, Menlo Park, CA, United States (U.S. corporation)
PI US 5763432 19980609
AI US 1997-794229 19970129 (8)
DT Utility
FS Granted
EXNAM Primary Examiner: Dees, Jose G.; Assistant Examiner: Badio, Barbara
LREP Reed, Dianne E.Bozicevic & Reed LLP
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 1700
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Novel compounds useful as inhibitors of estrone sulfatase are provided. The compounds have the structural formula (I) ##STR1## wherein X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine

dioxide ring, and the other various substituents are as defined herein. Pharmaceutical compositions and methods for using the compounds of formula (I) to treat estrogen-dependent disorders are provided as well.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **4954-12-5**
(preparation of steroid inhibitors of estrone sulfatase)
RN 4954-12-5 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

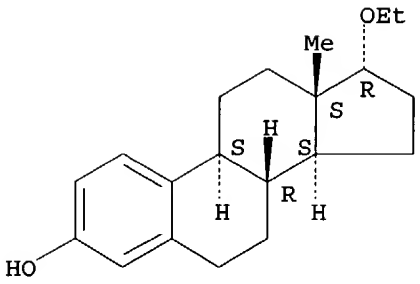
Absolute stereochemistry.



L60 ANSWER 5 OF 5 USPATFULL on STN
AN 96:82674 USPATFULL
TI Methods for neuroprotection
IN Simpkins, James W., Gainesville, FL, United States
Singh, Meharvan, Gainesville, FL, United States
Bishop, Jean, Jacksonville, FL, United States
PA University of Florida, Gainesville, FL, United States (U.S. corporation)
PI US 5554601 19960910
AI US 1994-318042 19941004 (8)
RLI Continuation-in-part of Ser. No. US 1993-149175, filed on 5 Nov 1993, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Weddington, Kevin E.
LREP Bromberg & Sunstein
CLMN Number of Claims: 29
ECL Exemplary Claim: 1
DRWN 11 Drawing Figure(s); 10 Drawing Page(s)
LN.CNT 1532
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB A method is provided for conferring neuroprotection on a population of cells using estrogen compounds that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compounds in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease so as to retard the adverse effects of these disorders, Examples of estrogen compounds that have insubstantial sex activity includes alpha isomers of estrogen compounds such as 17α estradiol.

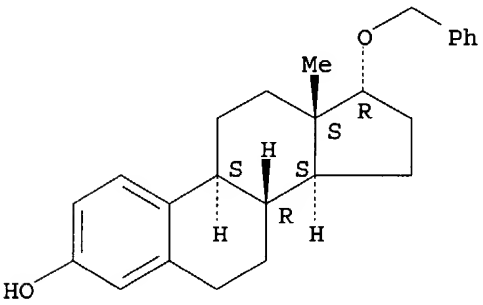
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **182624-49-3 182624-51-7 182823-27-4**
(methods for neuroprotection)
RN 182624-49-3 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



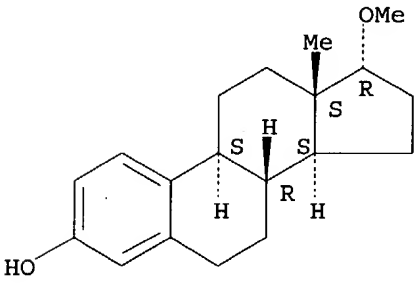
RN 182624-51-7 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 182823-27-4 USPATFULL
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FILE LAST UPDATED: 19 Jul 2004 (20040719/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L50 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:10439 HCAPLUS
DN 136:85991
ED Entered STN: 04 Jan 2002
TI Preparation of 17β-alkyl ether estradiol derivatives with cytoprotective activity of cells from degeneration through disease, trauma or aging
IN **Prokai, Laszlo; Simpkins, James W.**
PA University of Florida Research Foundation, Inc., USA
SO PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
FAN.CNT 1

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PI	WO 2002000619	A2	20020103	WO 2001-US41170	20010627 <--
	WO 2002000619	A3	20020829		
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	US 2002035100	A1	20020321	US 2001-893324	20010627 <--
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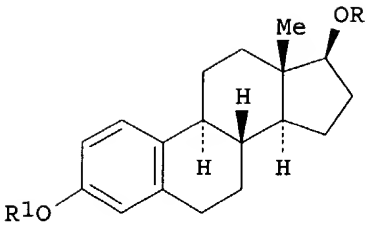
GI



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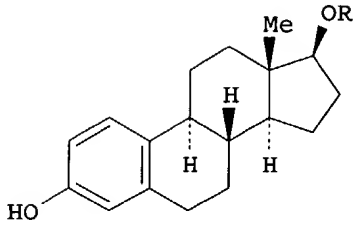


II

AB Cytoprotective compds. I (R = Me, Et, Pr, Bu, (CH2)5Me, or (CH2)7Me; R1 = OH) were prepared in 50-75% yields from 17β-estradiol. 17β-Estradiol and benzyl halide in K2CO3 gave 93% yield of 3-benzyloxyestra-1,3,5(10)-trien-17β-ol which was then alkylated with the appropriate alkyl halides in DMF and NaH yielding the 3-benzyloxy protected derivs. of I which were then deprotected via catalytic hydrogenation using ammonium formate in Pd/C. Thus compds. II (R = hexyl and octyl) were prepared in 70 and 75% resp., and were neuroprotective to a similar extent at a concentration of 10 μM and 1 μM. Typical compns. contain approx. 0.01-95% by weight of active ingredient and the percentage of active ingredient will depend upon the dosage form and mode of administration; an ED of the active agent as measured in the plasma of a subject may be in the range of 5pg/mL-5000pg/mL. Cytoprotective compds. I (R = OH; R1 = Bu, (CH2)7Me) were prepared from 17β-estradiol and Bu or octyl bromide in K2CO3 in 68 and 72% resp.

ST estradiol hydroxy alkylated deriv prepn cytoprotective compn; neuroprotective alkyl ether steroid prepn; crystal structure butoxyestratrienol

IT Steroids, preparation
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(alkylation of 17β-OH or 3-OH; preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Cytoprotective agents
(cardioprotective; preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Nervous system, disease
(degeneration; preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Alkylation
(hydroxyalkylation; preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Eye, disease
(macula, degeneration; preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Crystal structure
(of 17β-butoxyestra-1,3,5(10)-trien-3-ol)

IT Estrogen receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used as cytoprotective agents of cells from degeneration)

IT Anti-Alzheimer's agents
Anti-ischemic agents
Bone, disease
Drug delivery systems
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT Osteoporosis
(therapeutic agents; preparation of 17β- or 3-alkyl ether derivs. of

estradiol used for cytoprotective activity of cells from degeneration)

IT **319427-05-9P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

IT **4954-12-5P 21830-24-0P 128805-68-5P**
319427-03-7P 319427-04-8P 319427-06-0P
319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

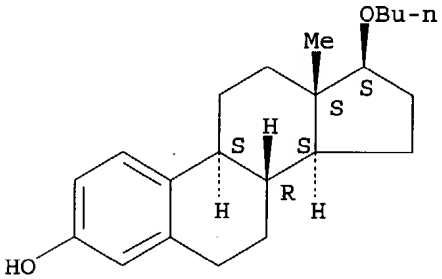
IT 50-28-2, 17β-Estradiol, reactions 109-65-9, Butyl bromide
111-83-1, Octyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT **14982-15-1P 141318-37-8P 319426-98-7P**
319426-99-8P 319427-00-4P 319427-01-5P
319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

IT **319427-05-9P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure)

RN 319427-05-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17β)- (9CI) (CA INDEX NAME)

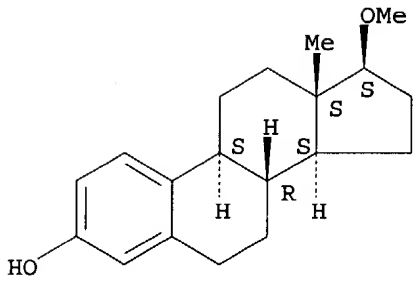
Absolute stereochemistry.



IT **4954-12-5P 21830-24-0P 128805-68-5P**
319427-03-7P 319427-04-8P 319427-06-0P
319427-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

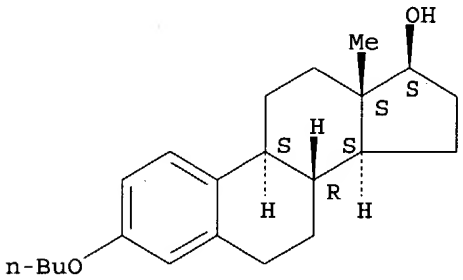
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



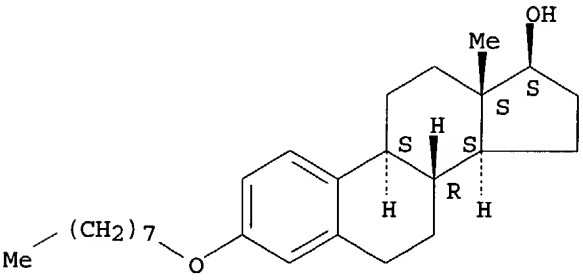
RN 21830-24-0 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-butoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



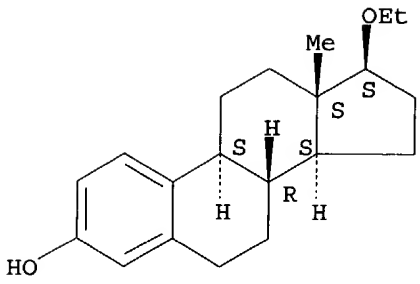
RN 128805-68-5 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-03-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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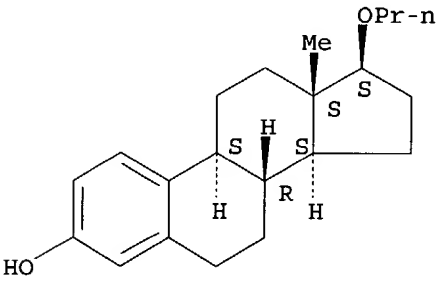
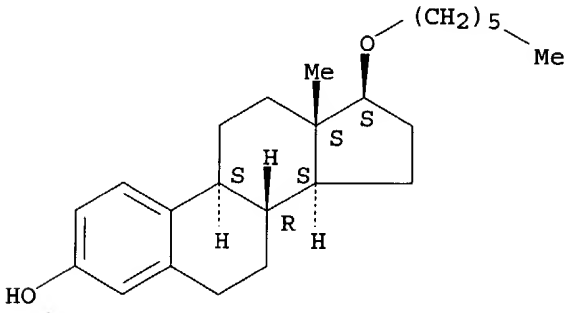
Absolute stereochemistry.



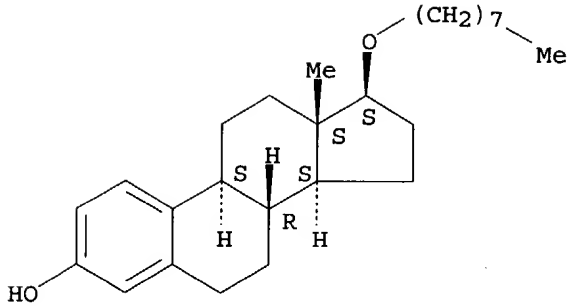
RN 319427-06-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-07-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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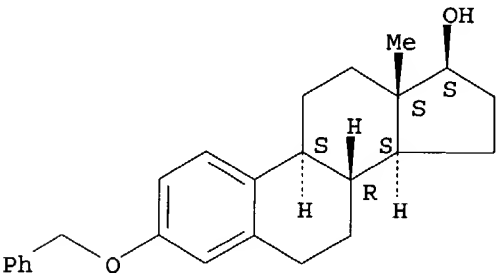
319426-99-8P 319427-00-4P 319427-01-5P
319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 17β- or 3-alkyl ether derivs. of estradiol used for cytoprotective activity of cells from degeneration)

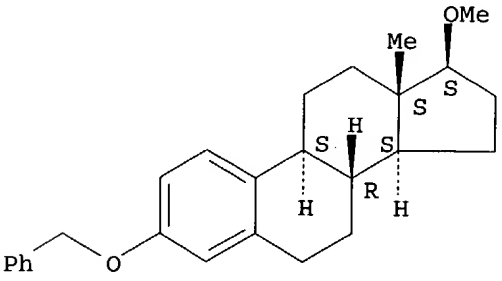
RN 14982-15-1 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 141318-37-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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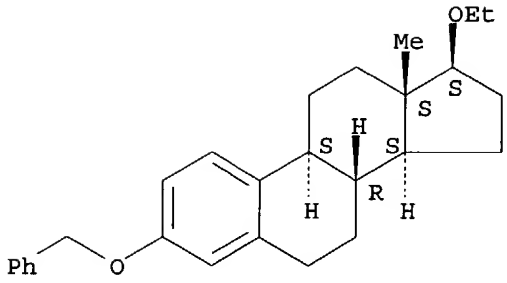
Absolute stereochemistry.



RN 319426-99-8 HCAPLUS
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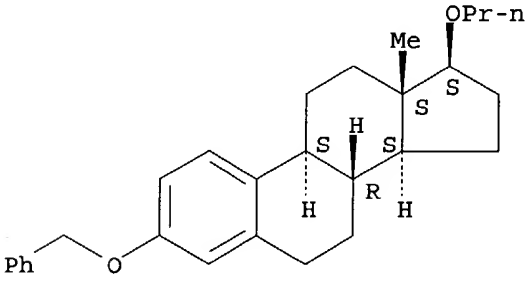
Absolute stereochemistry.



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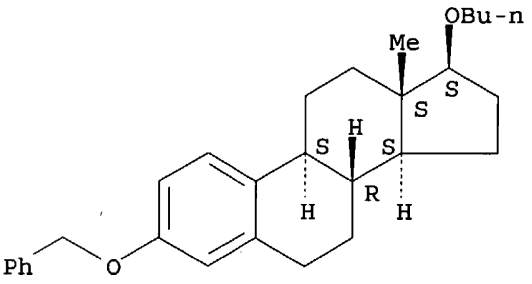
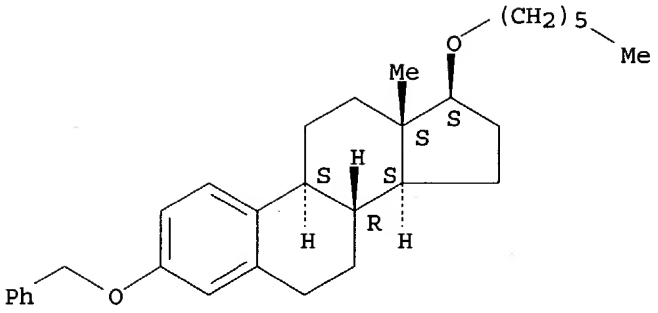
Absolute stereochemistry.



RN 319427-01-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-02-6 HCAPLUS
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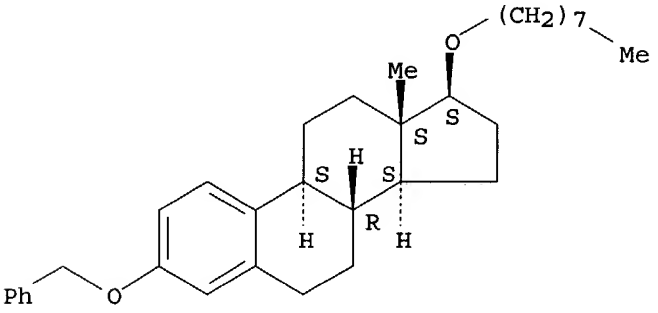
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:428147 HCAPLUS
DN 135:221441
ED Entered STN: 13 Jun 2001
TI Membrane fluidity effects of estratrienes
AU Liang, Y.; Belford, S.; Tang, F.; **Prokai, L.**; **Simpkins, J. W.**; Hughes, J. A.
CS Department of Pharmaceutics, University of Florida, Gainesville, FL, USA
SO Brain Research Bulletin (2001), 54(6), 661-668
CODEN: BRBUDU; ISSN: 0361-9230
PB Elsevier Science Inc.
DT Journal
LA English
CC 2-4 (Mammalian Hormones)
AB Estrogens have demonstrable neuroprotective effects. This fact has lead to the proposed use of estrogens for the prevention and/or treatment of Alzheimer's disease. The exact protective mechanism estrogens provide is not fully understood. In this report, a potential non-genomic mechanism for estratrienes involving alterations in membrane fluidity was studied. Steroids, such as estrogen, are known to be membrane-active and can alter the lipid packing. In this study the authors used fluorescent methodologies to address the effect of naturally occurring steroids (17α- and 17β-estradiol, testosterone, and progesterone) and new estratriene analogs on membrane fluidity using liposomes and HT-22 hippocampal cells. The study's results indicate steroids, based on the estratriene nucleus, can modulate lipid packing as evidenced by (1) decreased membrane fusion events and (2) decreased membrane fluidity. The effects on the membrane were both time- and concentration-dependent. It was also

demonstrated through rational design estratriene analogs can be synthesized with enhanced membrane effects. Finally, in a glutamate-induced toxicity HT-22 model, the authors also demonstrated cellular protection with the estratriene-based mols. and analogs. The data suggest the plethora of cellular actions of estrogens may relate to or be influenced by membrane effects of the steroid.

ST cell membrane fluidity estratriene; estradiol membrane fluidity

IT Animal cell line
(HT-22; estratrienes effects on membrane fluidity)

IT Membrane, biological
(bilayer; estratrienes effects on membrane fluidity)

IT Liposomes
(estratrienes effects on membrane fluidity)

IT Phosphatidylethanolamines, biological studies
Phosphatidylserines
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(estratrienes effects on membrane fluidity)

IT Brain
(hippocampus; estratrienes effects on membrane fluidity)

IT 57-88-5, Cholesterol, biological studies
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(estratrienes effects on membrane fluidity)

IT 50-28-2, 17β-Estradiol, biological studies 53-63-4, Estra-1,3,5(10)-trien-3-ol 57-83-0, Progesterone, biological studies 57-91-0, 17α-Estradiol 58-22-0, Testosterone
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(estratrienes effects on membrane fluidity)

IT **319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(estratrienes effects on membrane fluidity)

IT 50-50-0, 17β-Estradiol 3-benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(estratrienes effects on membrane fluidity)

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD

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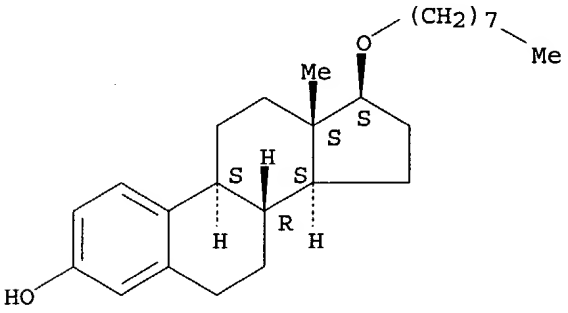
IT **319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(estratrienes effects on membrane fluidity)

RN 319427-07-1 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:114973 HCAPLUS

DN 134:158108

ED Entered STN: 15 Feb 2001

TI Methods of cytoprotection using an enantiomer of estrogen of ischemic damage

IN Covey, Douglas F.; **Simpkins, James W.**

PA University of Florida Research Foundation, Inc., USA; Apollo Biopharmaceutics Inc.; Washington University

SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K031-00

CC 2-4 (Mammalian Hormones)

Section cross-reference(s): 32

FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001010430	A2	20010215	WO 2000-US22163	20000811
	WO 2001010430	A3	20010830		
	WO 2001010430	C2	20020711		
	W: AU, CA, JP, KR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6350739	B1	20020226	US 1999-372627	19990811
	AU 2000069040	A5	20010305	AU 2000-69040	20000811
	EP 1143947	A2	20011017	EP 2000-957416	20000811
	EP 1143947	A3	20020911		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2003510336	T2	20030318	JP 2001-526632	20000811
PRAI	US 1999-372627	A	19990811		
	WO 2000-US22163	W	20000811		

AB The present invention in various embodiments provides methods of cytoprotection and treatment of disease that include providing an enantiomer of an estrogen compound to a population of cells in a subject with a cytodegenerative condition to protect those cells from further damage. The enantiomer of the invention is specifically, ent-17β-estradiol or ent-17β-estradiol 17-acetate. Examples of cytodegenerative conditions include stroke and neurodegenerative diseases. The invention further discloses a method of synthesis of ent-17β-estradiol and ent-17β-estradiol 17-acetate. A pharmaceutical formulation comprising an estrogen enantiomer in an oil is also claimed.

ST estrogen enantiomer prepn cytoprotection

IT Cytoprotective agents
(cardioprotective; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Brain, disease
(cerebrovascular, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Nervous system
(degeneration, treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(enantiomers; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Cytoprotective agents
(endothelial protection; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Heart, disease
(infarction, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)

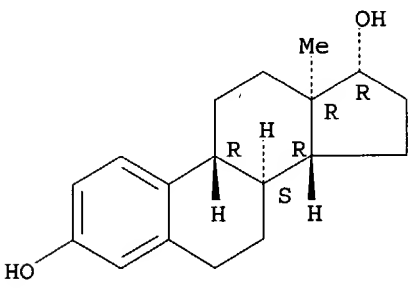
IT Surgery
(ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Anti-Alzheimer's agents
Anti-ischemic agents
Cytoprotective agents
(methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Cytoprotective agents
(neuroprotectants; methods of cytoprotection using synthetically prepared estrogen enantiomers)

IT Drug delivery systems
(oily; methods of cytoprotection using oily pharmaceutical formulations containing estrogen enantiomers)
IT Bone, disease
(osteodegenerative disease treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT Brain, disease
(stroke, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT Meninges
(subarachnoid hemorrhage, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT Injury
(trauma, ischemic event; methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT Osteoporosis
(treatment; methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT 300853-33-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT **3736-22-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT 139973-49-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT 4091-86-5P 185685-33-0P 325808-57-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
IT **3736-22-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(methods of cytoprotection using synthetically prepared estrogen enantiomers)
RN 3736-22-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (8α,9β,13α,14β,17.
alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:51133 HCAPLUS
DN 134:126193
ED Entered STN: 21 Jan 2001
TI The nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and a rat model of cerebral ischemia
AU Green, P. S.; Yang, S.-H.; Nilsson, K. R.; Kumar, A. S.; Covey, D. F.; **Simpkins, J. W.**
CS Center for the Neurobiology of Aging, University of Florida, Gainesville, FL, 32610, USA
SO Endocrinology (2001), 142(1), 400-406
CODEN: ENDOAO; ISSN: 0013-7227
PB Endocrine Society
DT Journal
LA English
CC 2-4 (Mammalian Hormones)
AB Estrogens are potent neuroprotective compds. in a variety of animal and cell culture models, and data indicate that estrogen receptor (ER)-mediated gene transcription is not required for some of these effects. To further address the requirement for an ER in estrogen enhancement of neuronal survival, the authors assessed the enantiomer of 17β-estradiol (Ent-E2), which has identical chemical properties but interacts only weakly with known ERs, for neuroprotective efficacy. Ent-E2 was both as potent and efficacious as 17β-estradiol in attenuating oxidative stress-induced death in HT-22 cells, a murine hippocampal cell line. Further, Ent-E2 completely attenuated H2O2 toxicity in human SK-N-SH neuroblastoma cells at a 10 nM concentration In a rodent model of focal ischemia, 17β-estradiol (100 μg/kg) or Ent-E2 (100 μg/kg), injected 2 h before middle cerebral artery occlusion, resulted in a 60 and 61% reduction in lesion volume, resp. Ent-E2, at the doses effective in this study, did not stimulate uterine growth or vaginal opening in juvenile female rats when administered daily for 3 days. These data indicate that the neuroprotective effects of estrogens, both in vitro and in vivo, can be disassocd. from the peripheral estrogenic actions.
ST estradiol enantiomer neuroprotectant cerebral ischemia
IT Brain
(hippocampus; nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT Brain, disease
(ischemia, focal; nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT Nerve
(neuron; nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT Cytoprotective agents
(neuroprotectants; nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT Oxidative stress, biological
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT Estrogens
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)

IT Estrogen receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT 7722-84-1, Hydrogen peroxide, biological studies
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
IT 50-28-2, 17β-Estradiol, biological studies **3736-22-9**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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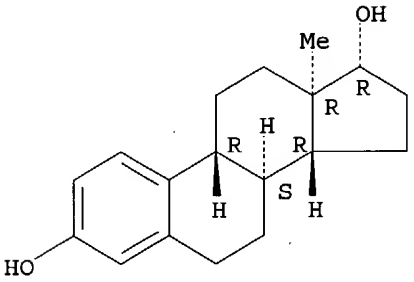
IT **3736-22-9**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nonfeminizing enantiomer of 17β-estradiol exerts protective effects in neuronal cultures and rat model of cerebral ischemia)
RN 3736-22-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (8α,9β,13α,14β,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:820327 HCAPLUS
DN 134:101056
ED Entered STN: 23 Nov 2000
TI Synthesis and Biological Evaluation of 17β-Alkoxyestra-1,3,5(10)-trienes as Potential Neuroprotectants Against Oxidative Stress
AU **Prokai, Laszlo**; Oon, Su-Min; Prokai-Tatrai, Katalin; Abboud, Khalil A.; **Simpkins, James W.**
CS Center for Drug Discovery College of Pharmacy Department of Anesthesiology College of Medicine and Center for Neurobiology of Aging College of Pharmacy, University of Florida, Gainesville, FL, 32610-0497, USA
SO Journal of Medicinal Chemistry (2001), 44(1), 110-114
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 32-3 (Steroids)
Section cross-reference(s): 1, 75
OS CASREACT 134:101056
AB 17β-O-Alkyl ethers (Me, Et, Pr, Bu, hexyl, and octyl) of estradiol were obtained from 3-O-benzyl-17β-estradiol with sodium hydride/alkyl halide, followed by the removal of the O-benzyl protecting group via catalytic transfer hydrogenation. An increase compared to estradiol in the protection of neural (HT-22) cells against oxidative stress due to exposure of glutamate was furnished by higher (C-3 to C-8) alkyl ethers, while Me and Et ethers decreased the neuroprotective effect significantly. Lipophilic (Bu and octyl) ethers blocking the phenolic hydroxyl (3-OH) of A-ring were inactive.
ST alkoxyestratriene prepn neuroprotectant oxidative stress; estratriene alkoxy prepn neuroprotectant oxidative stress
IT Cytoprotective agents
(neuroprotectants; synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
IT Crystal structure

Molecular structure
Oxidative stress, biological
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT Estrogens
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT **319427-05-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT **4954-12-5P 21830-24-0P 128805-68-5P**
319427-03-7P 319427-04-8P 319427-06-0P
319427-07-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT 50-28-2, 17β-Estradiol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

IT **14982-15-1P 141318-37-8P 319426-98-7P**
319426-99-8P 319427-00-4P 319427-01-5P
319427-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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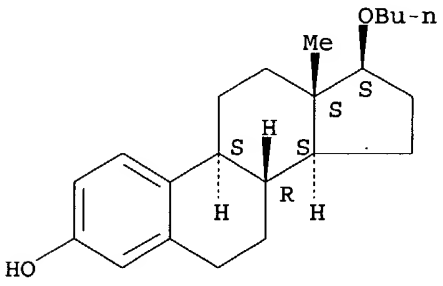
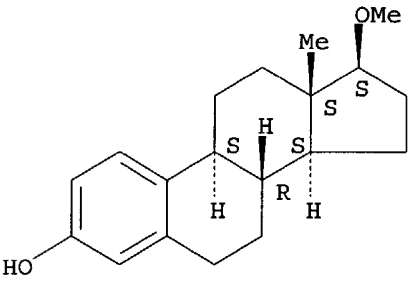
IT **319427-05-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 319427-05-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **4954-12-5P 21830-24-0P 128805-68-5P 319427-03-7P 319427-04-8P 319427-06-0P 319427-07-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 21830-24-0 HCAPLUS
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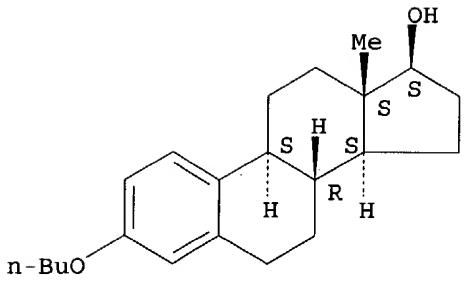
Absolute stereochemistry.



RN 128805-68-5 HCAPLUS
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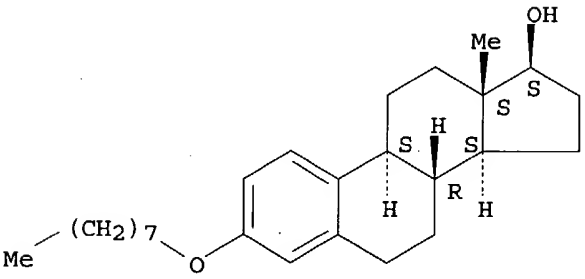
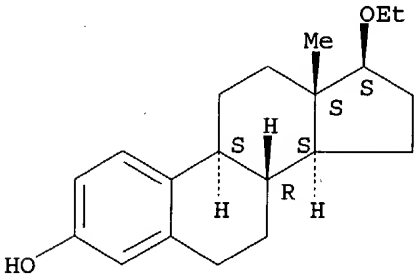
Absolute stereochemistry.



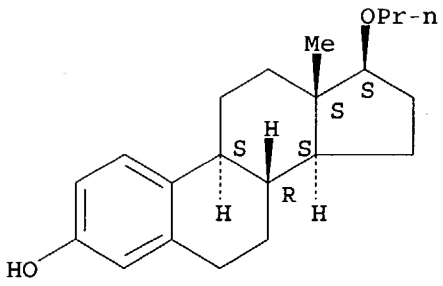
RN 319427-03-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



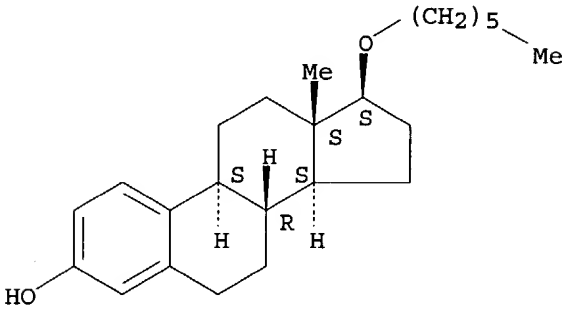
RN 319427-04-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



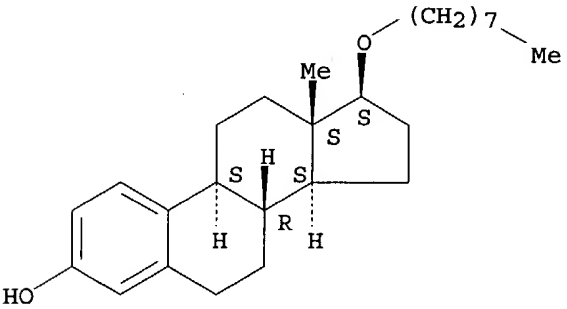
RN 319427-06-0 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



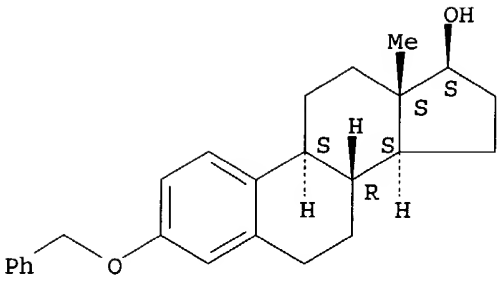
RN 319427-07-1 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



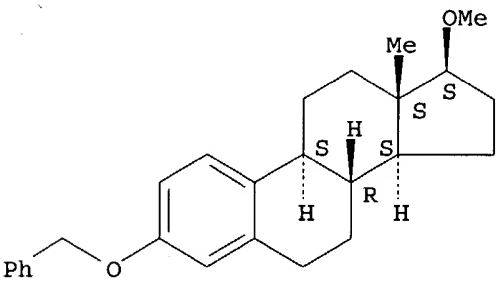
IT **14982-15-1P 141318-37-8P 319426-98-7P 319426-99-8P 319427-00-4P 319427-01-5P 319427-02-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. evaluation of 17β-alkoxyestra-1,3,5(10)-trienes as potential neuroprotectants against oxidative stress)
RN 14982-15-1 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



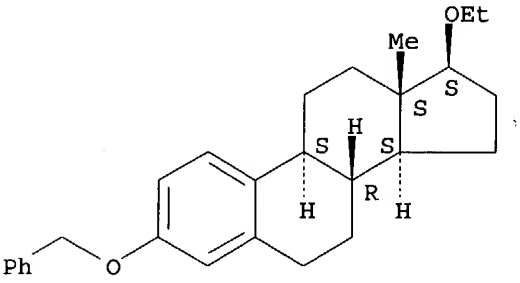
RN 141318-37-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



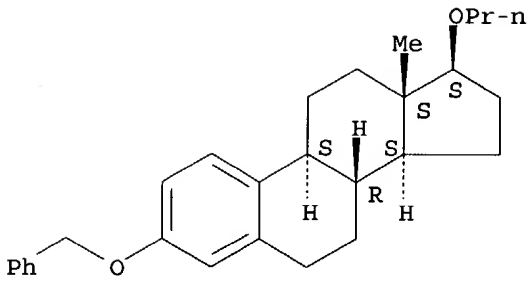
RN 319426-98-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



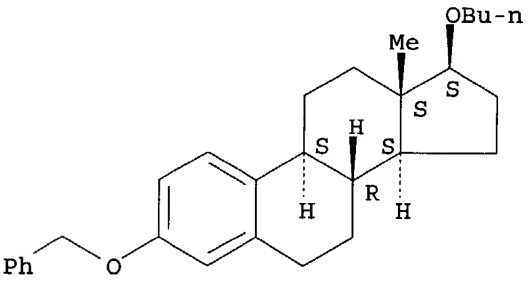
RN 319426-99-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



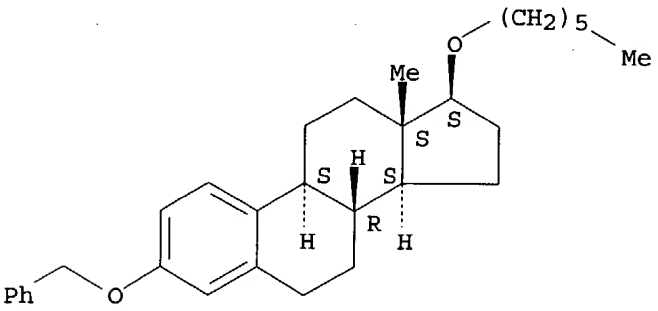
RN 319427-00-4 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



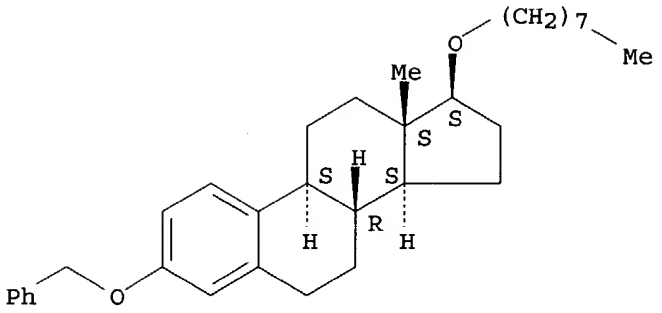
RN 319427-01-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 319427-02-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



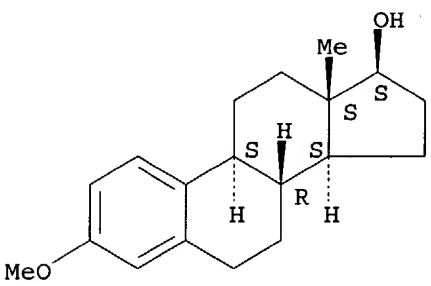
L50 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:204238 HCAPLUS
DN 126:195255
ED Entered STN: 28 Mar 1997
TI Use of non-estrogen polycyclic phenol compounds for the manufacture of a medicament for conferring neuroprotection to cells
IN **Simpkins, James W.**; Green, Patti S.; Gordon, Katherine
PA University of Florida Research Foundation, Incorporated, USA
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-00
ICS A61K031-05; A61K031-045; A61K031-11; A61K031-12; A61K031-56
CC 1-11 (Pharmacology)
Section cross-reference(s): 2
FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9703661	A1	19970206	WO 1996-US12146	19960724
	W: AU, CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2227634	AA	19970206	CA 1996-2227634	19960724
	AU 9665079	A1	19970218	AU 1996-65079	19960724
	EP 841906	A1	19980520	EP 1996-924692	19960724
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 11510144	T2	19990907	JP 1996-506961	19960724
	US 6197833	B1	20010306	US 1998-129209	19980804
PRAI	US 1995-1394P	P	19950724		
	US 1996-685574	A3	19960724		
	WO 1996-US12146	W	19960724		

AB Non-estrogen compds. having a terminal phenol group in a structure containing at least a second ring and having a mol. weight of less than 1000 Daltons (e.g. naphthols, phenanthrenes or steroids) are used for the manufacture of a medicament for conferring neuroprotection to cells in a subject.
ST polycyclic phenol deriv neuroprotectant
IT Nervous system
(degeneration; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT Structure-activity relationship
(neuroprotectant; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT Cytoprotective agents
(neuroprotectants; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT Anti-ischemic agents
(non-estrogen polycyclic phenol compds. for neuroprotectants)

IT Polycyclic compounds
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phenols; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT Phenols, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polycyclic; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT Amyloid
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(β-, Aβ 25-35, neurotoxicity from; non-estrogen polycyclic phenol compds. for neuroprotectants)
IT 52-39-1, Aldosterone 53-06-5, Cortisone 57-83-0, Progesterone, biological studies 57-88-5, Cholesterol, biological studies 58-22-0, Testosterone 72-33-3, Mestranol 108-95-2, Phenol, biological studies 128-37-0, Butylated hydroxytoluene, biological studies 130-79-0 521-18-6, Dihydrotestosterone **1035-77-4** 1474-53-9 1624-62-0 5976-67-0 15068-98-1 25013-16-5, Butylated hydroxyanisole
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(non-estrogen polycyclic phenol compds. for neuroprotectants)
IT 50-24-8, Prednisolone 50-27-1, Estriol 50-28-2, 3,17β-Estradiol, biological studies 53-16-7, Estrone, biological studies 53-63-4, Estra-1,3,5(10)-trien-3-ol 56-53-1 57-63-6, 17α-Ethynyl estradiol 57-91-0 83-43-2, 6α-Methylprednisolone 362-05-0 18839-90-2 104849-43-6 114549-37-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(non-estrogen polycyclic phenol compds. for neuroprotectants)
IT 85-01-8D, Phenanthrene, phenol group-containing derivs., biological studies 91-20-3D, Naphthalene, phenol group-containing derivs., biological studies 1321-67-1, Naphthol 29966-04-9D, Octahydrophenanthrene, phenol group-containing derivs. 51057-65-9, Phenanthrenemethanol 73493-69-3D, Tetrahydrophenanthrene, phenol group-containing derivs. 77468-40-7, Phenanthrenecarboxaldehyde
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(non-estrogen polycyclic phenol compds. for neuroprotectants)
IT **1035-77-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(non-estrogen polycyclic phenol compds. for neuroprotectants)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:580562 HCAPLUS
DN 125:294029
ED Entered STN: 30 Sep 1996
TI Methods for neuroprotection
IN **Simpkins, James W.**; Singh, Meharvan; Bishop, Jean
PA University of Florida, USA
SO U.S., 25 pp., Cont.-in-part of U.S. Ser. No. 149,175, abandoned.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
NCL 514182000
CC 2-4 (Mammalian Hormones)
FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5554601	A	19960910	US 1994-318042	19941004
	CA 2175603	AA	19950511	CA 1994-2175603	19941107
	WO 9512402	A1	19950511	WO 1994-US12782	19941107
	W: AU, CA, JP, KR				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9510901	A1	19950523	AU 1995-10901	19941107
	AU 699361	B2	19981203		
	EP 799041	A1	19971008	EP 1995-901795	19941107
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
	JP 11514327	T2	19991207	JP 1994-513454	19941107
	US 5843934	A	19981201	US 1996-648857	19960516
	US 5877169	A	19990302	US 1996-749703	19961115
	US 6319914	B1	20011120	US 1999-351492	19990712
	US 2003069217	A1	20030410	US 2002-82812	20020225
PRAI	US 1993-149175	B2	19931105		
	US 1994-318042	A	19941004		
	WO 1994-US12782	W	19941107		
	US 1996-648857	A2	19960516		
	US 1996-685574	A2	19960724		
	US 1996-749703	A3	19961115		
	US 1997-782883	A3	19970110		
	US 1998-128862	A3	19980804		
	US 1998-129209	A2	19980804		
	US 1998-179640	A3	19981027		
	US 1999-372627	A1	19990811		

AB A method is provided for conferring neuroprotection on a population of cells using estrogen compds. that have insubstantial sex activity and furthermore, a method is provided that utilizes estrogen compds. in the absence of testosterone for treating neurodegenerative diseases including Alzheimer's disease to retard the adverse effects of these disorders, Examples of estrogen compds. that have insubstantial sex activity includes alpha isomers of estrogen compds. such as 17α-estradiol.

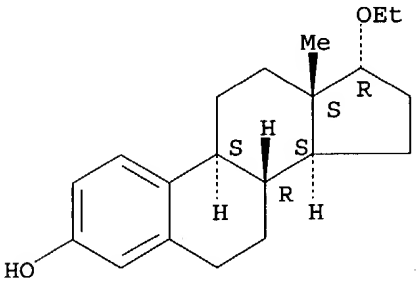
ST estrogen neuroprotection
IT Nerve
(methods for neuroprotection)
IT Estrogens
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)
IT Molecular structure-biological activity relationship
(neuroprotective; methods for neuroprotection)
IT Mental disorder
(Alzheimer's disease, methods for neuroprotection)
IT 53-16-7, biological studies 57-63-6, 17α-Ethynylestradiol
57-91-0, 17α-Estradiol 10093-54-6 15068-99-2 33602-53-8
65684-87-9 110114-70-0 **182624-49-3** 182624-50-6
182624-51-7 182624-52-8 182624-53-9 182624-54-0
182624-55-1 182624-56-2 182624-57-3 182624-58-4 182624-59-5

182624-60-8 182624-61-9 **182823-27-4**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)

IT **182624-49-3 182624-51-7 182823-27-4**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods for neuroprotection)

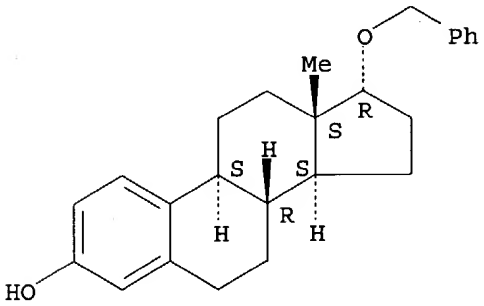
RN 182624-49-3 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



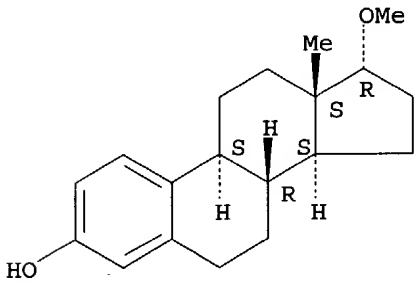
RN 182624-51-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 182823-27-4 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

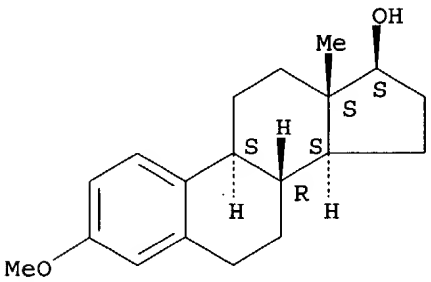
AN 1988:623419 HCAPLUS
DN 109:223419
ED Entered STN: 24 Dec 1988
TI Preparation and use of brain-specific dihydropyridine redox carrier-type derivatives of estrogenic agents for treating male sexual dysfunction
IN Anderson, Wesley R.; Bodor, Nicholas S.; **Simpkins, James W.**
PA University of Florida, USA
SO Eur. Pat. Appl., 60 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM A61K031-565
ICA A61K031-44
CC 2-10 (Mammalian Hormones)
Section cross-reference(s): 27
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 256668	A2	19880224	EP 1987-306224	19870714
	EP 256668	A3	19891004		
	EP 256668	B1	19921104		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4863911	A	19890905	US 1986-892861	19860804
	AT 81977	E	19921115	AT 1987-306224	19870714
	AU 8776308	A1	19880211	AU 1987-76308	19870730
	AU 603368	B2	19901115		
	CA 1300020	A1	19920505	CA 1987-543611	19870803
	JP 63099095	A2	19880430	JP 1987-195140	19870804
	JP 2646568	B2	19970827		
PRAI	US 1986-892861		19860804		
	EP 1987-306224		19870714		

OS MARPAT 109:223419
AB Compds. E-DHC or E-[DHC]n [E = estrogen or estrogen with reactive OH group(s); DHC = reduced, biooxidizable, blood-brain barrier-penetrating, lipoidal form of a dihydropyridine-pyridinium salt redox carrier; n = number of reactive OH groups] or nontoxic pharmaceutically acceptable salts are used to prepare a medication for treating male sexual dysfunction. 17β-[(1-Methyl-1,4-dihydro-3-pyridinyl)carbonyloxy]estra-1,3,5(10)-trien-3-ol (I) was prepared from estradiol and nicotinoyl chloride hydrochloride in 4 steps. Bilaterally orchidectomized adult male Sprague-Dawley rats were injected with I (3 mg/kg in DMSO). The animals responded with a decrease in mounting and intromission latencies by 3 days which persisted for >28 days. Intromission frequencies increased by 300% over castrate levels through 14 days and were restored to precastrate levels through 4 wk.
ST estrogen dihydropyridine conjugate male sexual dysfunction
IT Steroids, compounds
RL: BIOL (Biological study)
(1,3,5(10)-triunsatd., hydroxy, conjugates, with dihydropyridine redox carriers, for treating male sexual dysfunction)
IT Sex
(activity, disorder, male, treatment of, by estrogen-dihydropyridine redox carrier conjugates)
IT Estrogens
RL: BIOL (Biological study)
(conjugates, with dihydropyridine redox carriers, for treatment of male sexual dysfunction)
IT 50-27-1D, Estriol, dihydropyridine redox carrier conjugates 50-28-2D, Estradiol, dihydropyridine redox carrier conjugates 50-50-0D, Estradiol benzoate, dihydropyridine redox carrier conjugates 53-16-7D, Estrone, dihydropyridine redox carrier conjugates 57-63-6D, Ethinyl estradiol, dihydropyridine redox carrier conjugates 72-33-3D, Mestranol, dihydropyridine redox carrier conjugates 152-43-2D, Quinestrol,

dihydropyridine redox carrier conjugates 313-06-4D, Estradiol cypionate, dihydropyridine redox carrier conjugates 979-32-8D, Estradiol valerate, dihydropyridine redox carrier conjugates 3571-53-7D, Estradiol undecylate, dihydropyridine redox carrier conjugates 3758-34-7D, dihydropyridine redox carrier conjugates 4956-37-0D, Estradiol enanthate, dihydropyridine redox carrier conjugates 5941-36-6D, Estrazinol, dihydropyridine redox carrier conjugates 10322-73-3D, dihydropyridine redox carrier conjugates 27790-75-6D, Dihydropyridine, derivs., estrogen conjugates 39791-20-3D, Nylestriol, dihydropyridine redox carrier conjugates 47703-84-4D, dihydropyridine redox carrier conjugates 117539-14-7D, estrogens conjugates
RL: BIOL (Biological study)
(male sexual dysfunction treatment by)
IT 4248-62-8P 4248-63-9P 20260-53-1P, Nicotinoyl chloride hydrochloride 104117-66-0P 106146-62-7P 106146-63-8P 106146-65-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of estrogen-dihydropyridine redox
carrier conjugates for treating male sexual dysfunction)
IT 103562-82-9P
RL: PREP (Preparation)
(preparation of and male sexual dysfunction treatment by)
IT 106146-61-6P 106146-64-9P 106146-66-1P 106146-67-2P
RL: PREP (Preparation)
(preparation of, for treating male sexual dysfunction)
IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 59-67-6, Nicotinic acid, reactions **1035-77-4**, Estradiol-3-methyl ether 7719-09-7, Thionyl chloride 117539-15-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of estrogen-dihydropyridine redox carrier conjugates for treating male sexual dysfunction)
IT **1035-77-4**, Estradiol-3-methyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of estrogen-dihydropyridine redox carrier conjugates for treating male sexual dysfunction)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L50 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:27813 HCAPLUS
DN 106:27813
ED Entered STN: 07 Feb 1987
TI Method and compositions for weight control
IN Bodor, Nicholas S.; Estes, Kerry S.; **Simpkins, James W.**
PA University of Florida, USA
SO U.S., 33 pp.

CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-58
NCL 514176000
CC 1-10 (Pharmacology)
Section cross-reference(s): 32
FAN.CNT 1

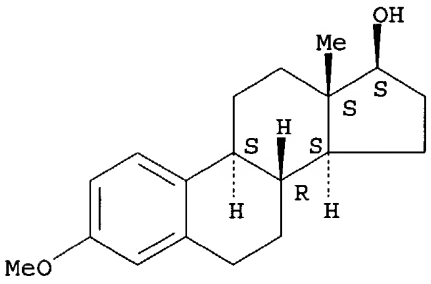
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4617298	A	19861014	US 1985-790159	19851022
	AU 8663425	A1	19870430	AU 1986-63425	19861001
	EP 220844	A2	19870506	EP 1986-307536	19861001
	EP 220844	A3	19890830		

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

PRAI US 1985-790159 19851022
OS CASREACT 106:27813
AB A method is given for controlling mammalian body weight by administration of E-DHC where E is an estrogen and DHC is the reduced, biooxidizable, blood-brain barrier penetrating, lipoidal form of a dihydropyridine.dblarw.pyridinium salt redox carrier. A preferred compound is the estrdiol derivative 17β-[(1-methyl-1,4-dihydro-3-pyridinyl)carbonyloxy]estra-1,3,5(10)-trien-3-ol (I). Thus, administration of 1-5 mg I/kg to female rats caused weight loss with little effect on the estrous cycle. The synthesis of the compds. is given.
ST estrogen pyridinyl prepn antiobesity agent
IT Estrogens
RL: BIOL (Biological study)
(dihydropyridine redox-type derivs., as antiobesity agents)
IT Antiobesity agents
(estrogen dihydropyridine redox-type derivs.)
IT 59-67-6, Nicotinic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of estrone via acid chloride)
IT 50-28-2, biological studies 53-16-7, Estrone, reactions
1035-77-4, Estradiol 3-methyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with nicotinoyl chloride)
IT 106146-62-7P 106146-63-8P 106146-64-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dithionite reduction of)
IT 20260-53-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification by, of estrogens)
IT 4248-62-8P 4248-63-9P 104117-66-0P 106146-65-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and quaternization of, with Me iodide)
IT 106146-61-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective hydrolysis of)
IT 106146-66-1P 106146-67-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as body weight-reducing agent)
IT 103562-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, with body weight-reducing agent)
IT 74-88-4, Methyl iodide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of estrone nicotinate)

IT **1035-77-4**, Estradiol 3-methyl ether
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with nicotinoyl chloride)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> => d all hitstr tot l59

L59 ANSWER 1 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:974249 HCAPLUS
DN 138:44718
ED Entered STN: 26 Dec 2002
TI Extended-release growth promoting two component composition
IN Cady, Susan Mancini; Macar, Claude; Gibson, John W.
PA Akzo Nobel N.V., Neth.; Southern Biosystems
SO U.S., 10 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-56
ICS A61K031-335; C07J001-00; C07D313-08
NCL 514170000; 514171000; 514178000; 514182000; 514450000; 552625000; 552646000; 552650000; 549269000
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 18
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6498153	B1	20021224	US 1999-273862	19990322 <--
PRAI FR 1998-16707	A	19981231 <--		

OS MARPAT 138:44718
AB An extended-release composition comprising a first composition comprising growth promoters and a second composition comprising growth promoters and a biodegradable polymer is described. A method of increasing weight gain in food animals utilizing the composition, a pharmaceutical dosage form containing the composition and a method of preparing the pharmaceutical dosage form are also described, as are pellets of the composition for implantation in food animals. For example, 1000 g of a mixture of 17β-acetoxy-4,9,11-trien-3-one and estra-1,3,5(10)-trien-3,17β-diol, also containing cholesterol, Et cellulose and magnesium stearate, was granulated with 52.6 g of 75:25 DL-lactide-glycolide copolymer. The dried, sieved granulation was tableted to provide pellets with an average weight of about 33 mg and an average hardness of about 70 N. Pellets were then coated with

DL-lactide-glycolide copolymer (65:25 or 75:25, resp.).
ST growth promoter biodegradable polymer pellet controlled release implant; farm animal growth promoter controlled release implant
IT Polymers, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biodegradable; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Polyesters, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(dilactone-based; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Polyesters, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(glycolide-based; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Drug delivery systems
(implants, controlled-release; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Polyesters, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lactide; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Glass transition temperature
Livestock
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Growth factors, animal
RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT Drug delivery systems
(pellets; pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT 50-28-2, Estra-1,3,5(10)-triene-3,17-diol (17β)-, biological studies 57-83-0, Pregn-4-ene-3,20-dione, biological studies 57-85-2, 17β-Propionyloxy-4-androsten-3-one 10109-77-0 10161-34-9, 17β-Acetoxyestra-4,9,11-trien-3-one 55331-29-8 **55561-42-7**
RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
IT 26009-03-0, Polyglycolide 26023-30-3, Poly[oxy(1-methyl-2-oxo-1,2-ethanediyl)] 26161-42-2 26202-08-4, Polyglycolide 26680-10-4, Poly(DL-lactide) 26780-50-7, Glycolide-DL-lactide copolymer 30846-39-0, Glycolide-L-lactide copolymer 33135-50-1, Poly(L-lactide)
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; GB 2167662 A 1986 HCAPLUS
(2) Boswell; US 3773919 A 1973 HCAPLUS
(3) Brown; US 4393041 A 1983 HCAPLUS
(4) Deasy, P; International Journal of Pharmaceutics 1993, V89, P251 HCAPLUS
(5) Dirix; US 5389379 A 1995 HCAPLUS
(6) Foutz, C; Journal of Animal Science 1997, V75, P1256 HCAPLUS
(7) Grandadam; US 3939265 A 1976 HCAPLUS
(8) Hendricks, D; Journal of Animal Science 1997, V75, P2627
(9) Herbert; US 5654008 A 1997 HCAPLUS
(10) Hwang, R; Drug Development and Industrial Pharmacy 1993, V19, P507 HCAPLUS
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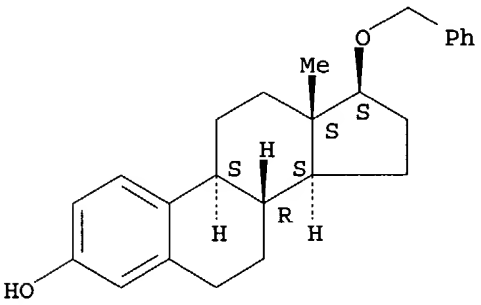
(12) Lee; US 5629008 A 1997 HCAPLUS
(13) Lewis; US 5288496 A 1994
(14) Macvinish, L; Animal Products 1988, V47, P75 HCAPLUS
(15) Nuwayser; US 4624665 A 1986 HCAPLUS
(16) Reul; US 4331651 A 1982 HCAPLUS
(17) Tice; US 5407609 A 1995

IT **55561-42-7**
RL: AGR (Agricultural use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pellets containing growth promoters and biodegradable polymers for controlled-release implants for farm animals)

RN 55561-42-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 2 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:30570 HCAPLUS
DN 130:293190
ED Entered STN: 15 Jan 1999
TI Human 17β-hydroxysteroid dehydrogenase-ligand complexes: crystals of different space groups with various cations and combined seeding and co-crystallization
AU Zhu, D.-W.; Han, Q.; Qiu, W.; Campbell, R. L.; Xie, B.-X.; Azzi, A.; Lin, S.-X.
CS CHUL Research Center, Medical Research Council Group in Molecular Endocrinology, Laval University, Quebec, G1V 4G2, Can.
SO Journal of Crystal Growth (**1999**), 196(2-4), 356-364
CODEN: JCRGAE; ISSN: 0022-0248
PB Elsevier Science B.V.
DT Journal
LA English
CC 7-5 (Enzymes)
Section cross-reference(s): 75
AB Human estrogenic 17β-hydroxysteroid dehydrogenase (17β-HSD1) is responsible for the synthesis of active estrogens that stimulate the proliferation of breast cancer cells. The enzyme has been crystallized using a Mg2+/PEG (3500)/β-octyl glucoside system. The space group of these crystals is C2. Here we report that cations can affect 17β-HSD1 crystallization significantly. In the presence of Mn2+ instead of Mg2+, crystals have been obtained in the same space group with similar unit cell dimensions. In the presence of Li+ and Na+ instead of Mg2+, the space group has been changed to P212121. A whole data set for a crystal of 17β-HSD1 complex with progesterone grown in the presence of Li+ has been collected to 1.95 Å resolution with a synchrotron source. The cell dimensions are a=41.91 Å, b=108.21 Å, c=117.00 Å. The structure has been preliminarily determined by mol. replacement, yielding

important information on crystal packing in the presence of different cations. In order to further understand the structure-function relationship of 17β-HSD1, enzyme complexes with several ligands have been crystallized As the steroids have very low aqueous solubility, we used a combined method of seeding and co-crystallization to obtain crystals of 17β-HSD1 complexed with various ligands. This method provides ideal conditions for growing complex crystals, with ligands such as 20α-hydroxysteroid progesterone, testosterone and 17β-methyl-estradiol-NADP+. Several complex structures have been determined with reliable electronic d. of the bound ligands.

ST hydroxysteroid dehydrogenase ligand complex crystn human; crystal structure hydroxysteroid dehydrogenase ligand complex human

IT Cations
Crystal growth
Crystal structure
(crystals of human 17β-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

IT 9028-61-9, 17β-Estradiol dehydrogenase
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(crystals of human 17β-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

IT 53-59-8DP, Nadp, complexes with 17β-hydroxysteroid dehydrogenase and 17β-methylestradiol 58-22-0DP, Testosterone, complexes with 17β-hydroxysteroid dehydrogenase 145-14-2DP, 20α-HydroxyProgesterone, complexes with 17β-hydroxysteroid dehydrogenase **4954-12-5DP**, complexes with 17β-hydroxysteroid dehydrogenase and NADP 9028-61-9DP, 17β-Estradiol dehydrogenase, ligand complexes
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(crystals of human 17β-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Azzi, A; Nature Struct Biol 1996, V3, P665 HCAPLUS
(2) Breton, R; J Steroid Biochem Mol Biol 1994, V50, P275 HCAPLUS
(3) Breton, R; Structure 1996, V8, P905
(4) Chin, C; Steroid 1973, V22, P373 HCAPLUS
(5) Crosio, M; J Mol Biol 1992, V228, P243 HCAPLUS
(6) Descomps, B; Bull Soc Chim Biol 1968, V50, P1681 HCAPLUS
(7) Geissler, W; Nat Genet 1994, V7, P34 HCAPLUS
(8) Ghosh, D; Structure 1995, V5, P503
(9) Han, Q; J Crystal Growth 1996, V168, P181 HCAPLUS
(10) Jarabak, J; Methods Enzymol 1969, V15, P746 HCAPLUS
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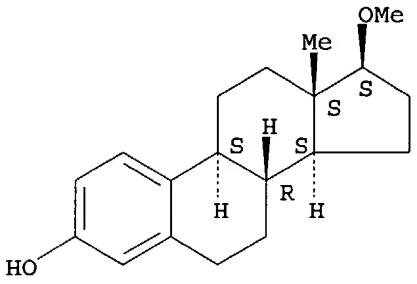
(18) Murdock, G; Biochemistry 1986, V25, P641 HCAPLUS
(19) Otwinowski, M; Methods in Enzymology 1996, P276
(20) Peltoketo, H; FEBS Lett 1988, V239, P73 HCAPLUS
(21) Poulin, R; Cancer Res 1986, V46, P4933 HCAPLUS
(22) Stura, E; Crystallization of Nucleic Acids and proteins 1992, P99 HCAPLUS
(23) Wu, L; J Biol Chem 1993, V268, P12964 HCAPLUS
(24) Zhu, D; Acta Crystallogr D 1994, V50, P550
(25) Zhu, D; J Crystal Growth 1996, V168, P272
(26) Zhu, D; J Mol Biol 1993, V234, P242 HCAPLUS

IT **4954-12-5DP**, complexes with 17β-hydroxysteroid dehydrogenase and NADP

RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(crystals of human 17β-hydroxysteroid dehydrogenase-ligand complexes have different space groups with various cations)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

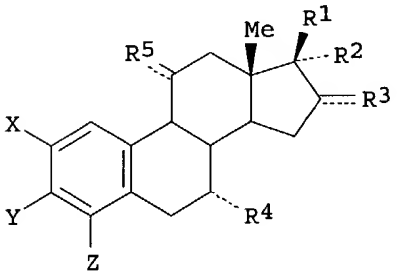
Absolute stereochemistry.



L59 ANSWER 3 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:397783 HCAPLUS
DN 129:54482
ED Entered STN: 29 Jun 1998
TI Preparation of steroid inhibitors of estrone sulfatase and associated pharmaceutical compositions and methods of use
IN Tanabe, Masato; Peters, Richard H.; Chao, Wan-ru; Shigeno, Kazuhiko
PA SRI International, USA
SO U.S., 23 pp.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-58
ICS C07J071-00
NCL 514176000
CC 32-3 (Steroids)
Section cross-reference(s): 1, 2
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5763432	A	19980609	US 1997-794229	19970129 <--
	US 5861388	A	19990119	US 1997-1601	19971231 <--
	WO 9832763	A1	19980730	WO 1998-US1846	19980129 <--

W: CA, JP, KR
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRAI US 1997-794229 19970129 <--
OS MARPAT 129:54482
GI



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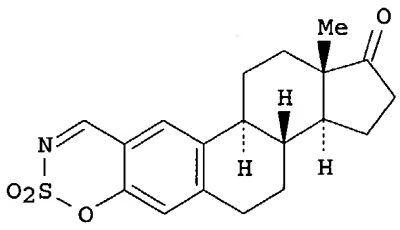


II

AB Estratriene derivs. of formula I [X and Y, or Y and Z, form an oxathiazine dioxide ring or a dihydro-oxathiazine dioxide ring; R1, R2 = H, alkyl, alkynyl, (substituted) OH; R1R2 = O, S, (substituted) CH2; R3 = H, halo, alkyl, CH2; R4 = H, alkyl; R5 = H, OH, alkyl, alkenyl, alkoxy, aryl, CH2] are prepared as inhibitors of estrone sulfatase. Pharmaceutical compns. and methods for using I to treat estrogen-dependent disorders are provided as well. Thus, estradiol is transformed into II in 3 steps. In an estrone sulfatase inhibition assay, II showed 5-% inhibition at 9.3 nM.

ST estratriene deriv prepn estrone sulfatase inhibitor

IT 208758-20-7P 208758-22-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)

IT 208758-16-1P 208758-17-2P 208758-21-8P 208758-23-0P 208758-25-2P
208758-33-2P 208758-34-3P 208758-35-4P 208758-36-5P 208758-37-6P
208758-38-7P 208758-39-8P 208758-41-2P 208758-43-4P 208758-48-9P
208758-52-5P 208758-54-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of steroid inhibitors of estrone sulfatase)

IT 59298-96-3, Estrone sulfatase
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of steroid inhibitors of estrone sulfatase)

IT 50-28-2, Estradiol, reactions 53-16-7, Estrone, reactions 57-63-6, 17α-Ethynylestradiol 1530-32-1, Ethyltriphenylphosphonium bromide 1779-51-7, Butyltriphenylphosphonium bromide **4954-12-5** 6228-47-3, Propyltriphenylphosphonium bromide 7678-95-7 59077-04-2, 19-Norpregna-1,3,5(10)-trien-3-ol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 4736-62-3P 6599-97-9P 13879-55-5P 13879-56-6P 31559-62-3P
34111-53-0P 57711-40-7P 64215-82-3P 99898-93-8P 120574-27-8P
120574-28-9P 123715-79-7P 137352-12-6P 206442-55-9P 208758-18-3P
208758-19-4P 208758-24-1P 208758-26-3P 208758-27-4P 208758-28-5P
208758-29-6P 208758-30-9P 208758-31-0P 208758-32-1P 208758-40-1P
208758-42-3P 208758-44-5P 208758-45-6P 208758-46-7P 208758-47-8P
208758-50-3P 208758-51-4P 208758-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

IT 208758-49-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of steroid inhibitors of estrone sulfatase)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Babcock; US 4297350 1981 HCAPLUS

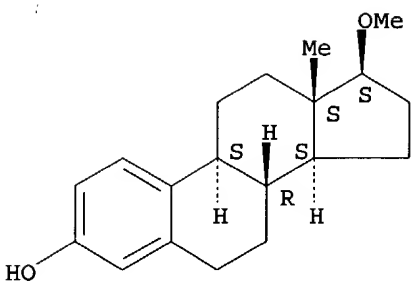
(2) Kuehne; US 3033860 1962 HCAPLUS

IT **4954-12-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of steroid inhibitors of estrone sulfatase)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

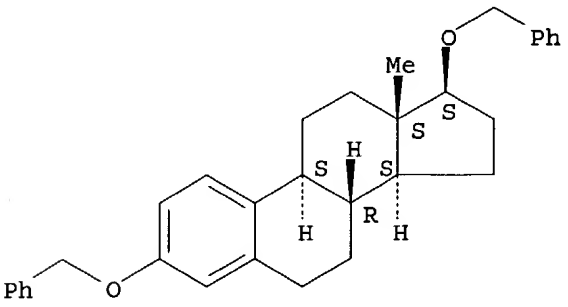
Absolute stereochemistry.



L59 ANSWER 4 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:570477 HCAPLUS
DN 117:170477
ED Entered STN: 01 Nov 1992
TI Aluminum chloride - N,N-dimethylaniline: a novel benzyl and allyl ether cleavage reagent
AU Akiyama, Takahiko; Hirofuji, Hajimu; Ozaki, Shoichiro
CS Fac. Eng., Ehime Univ., Matsuyama, 790, Japan
SO Bulletin of the Chemical Society of Japan (**1992**), 65(7), 1932-8
CODEN: BCSJA8; ISSN: 0009-2673
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 117:170477
AB A combination system of AlCl3-N,N-dimethylaniline was found to cleave benzyl ethers readily to give parent alcs. in excellent yields. The system also cleaved allyl as well as Me ethers. Numerous functional groups such as benzoyloxy, phenylthio, and olefinic double bond were not affected. Comparisons of AlCl3-N,N-dimethylaniline and AlCl3-anisole were described.
ST aluminum trichloride dimethylaniline cleavage ether; benzyl ether cleavage aluminum trichloride dimethylaniline; allyl ether cleavage aluminum trichloride dimethylaniline; aniline dimethyl aluminum trichloride cleavage ether
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(allyl, cleavage of, with aluminum chloride and dimethylaniline)
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzyl, cleavage of, with aluminum trichloride and dimethylaniline)
IT 78-89-7, 2-Chloro-1-propanol 4799-68-2, 3-(Benzyloxy)-1-propanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzoylation of)
IT 2550-26-7, 4-Phenyl-2-butanone
RL: RCT (Reactant); RACT (Reactant or reagent)
(borohydride reduction of)
IT 121-69-7, N,N-Dimethylaniline, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage by aluminum trichloride and, benzyl and allyl ethers)
IT 100-66-3, Anisole, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage by aluminum trichloride and, of benzyl and allyl ethers)
IT 108-95-2, Phenol, reactions 701-56-4, p-Methoxy-N,N-dimethylaniline 15799-79-8, m-Methoxy-N,N-dimethylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage by aluminum trichloride and, of benzyl phenylpropyl ether)
IT 7646-78-8, Tin tetrachloride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage by anisole and, of benzyl phenylpropyl ether)

IT 7446-70-0, Aluminum trichloride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage by dimethylaniline and, of benzylallyl ethers)
IT 1981-90-4 67685-90-9 108741-19-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(ether cleavage of, with aluminum trichloride and dimethylaniline)
IT 100-02-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with benzyl chloropropyl ether)
IT 70770-06-8P, Benzyl 3-phenylpropyl ether
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cleavage of, with aluminum trichloride and dimethylaniline)
IT 2046-33-5P, Methyl 3-phenylpropyl ether 6793-92-6P, Benzyl 4-bromophenyl ether 7278-60-6P 64740-44-9P **69455-04-5P** 69483-57-4P 93981-51-2P 96154-40-4P 101747-16-4P 133992-66-2P 143703-94-0P 143703-95-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ether cleavage of, with aluminum trichloride and dimethylaniline)
IT 122-97-4P, 3-Phenylpropanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of)
IT 50-28-2P, Estra-1,3,5(10)-triene-3,17-diol (17β)-, preparation 57-88-5P, Cholest-5-en-3-ol (3β)-, preparation 80-97-7P 106-22-9P 106-41-2P 834-14-0P 883-90-9P 2344-70-9P 2722-36-3P, 3-Phenyl-1-butanol 3204-68-0P 6946-99-2P 24536-40-1P **55561-42-7P** 66971-02-6P 104330-36-1P 131335-38-1P 131432-84-3P 143703-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 26420-79-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, etherification of, with nitrophenol and phenylsulfenylation of)
IT **69455-04-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and ether cleavage of, with aluminum trichloride and dimethylaniline)
RN 69455-04-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

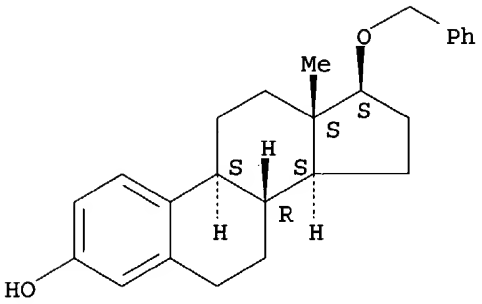
Absolute stereochemistry.



IT **55561-42-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 55561-42-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA

INDEX NAME)

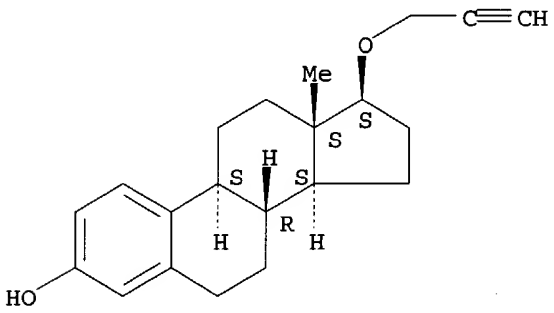
Absolute stereochemistry.



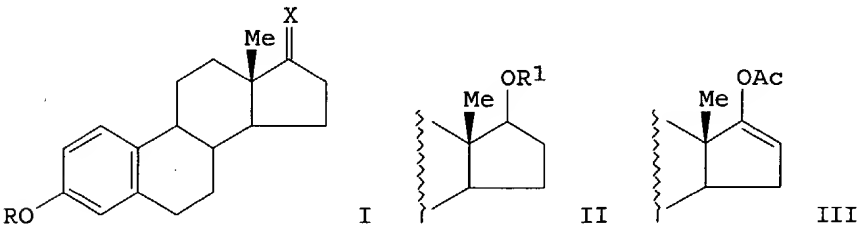
L59 ANSWER 5 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:408261 HCAPLUS
DN 117:8261
ED Entered STN: 11 Jul 1992
TI Synthesis of o-carboranylmethyl ethers of steroids as potential target substrates for boron neutron capture therapy
AU Schneiderova, Lenka; Strouf, Oldrich; Gruner, Bohumir; Pouzar, Vladimir; Drasar, Pavel; Hampl, Richard; Kimlova, Irena
CS Int. Inorg. Chem., Czech. Acad. Sci., Prague, 160 00, Czech.
SO Collection of Czechoslovak Chemical Communications (**1992**), 57(3), 463-71
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 32-3 (Steroids)
AB o-Carboranylmethyl ethers of steroids were synthesized by insertion of steroidal 2-propynyloxy derivs. into 6,9-bis(acetonitrile)decaborane(12). This reaction afforded compds. with estrane and androstane skeleton, potentially useful in boron neutron capture therapy of hormone-sensitive forms of cancer, i.e., 17β-o-carboranylmethyl ether of estradiol (I) (yield 14%) and 3β- and 17β-carboranylmethyl ethers of androstenediol (yield 12% and 13%, resp.). Jones oxidation afforded carboranyl derivative of androsten-17-one in 75% yield. As shown by a study of the insertion reaction of 3β-(2-propynyloxy)cholest-5-ene, the low yields of the insertion reaction cannot be increased by changing the reaction conditions. The relative binding affinity of I to estrogen receptors from rat uterine and human breast tumor cytosol was 3.0 and 0.29% resp., of that of estradiol.
ST carboranylmethyl ether steroid; estrogen receptor binding carboranylmethoxyestrol
IT Receptors
RL: RCT (Reactant); RACT (Reactant or reagent)
(estrogen, binding by, of estradiol carboranylmethyl ether)
IT Estrogens
RL: RCT (Reactant); RACT (Reactant or reagent)
(receptors, binding by, of estradiol carboranylmethyl ether)
IT 141887-27-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and binding of, to estrogen receptors)
IT 141870-63-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
IT 138473-74-2P 141870-64-6P 141887-25-4P 141887-26-5P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
IT 126003-29-0 126003-37-0 126003-41-6 **126003-44-9**
126003-45-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carborane derivative)
IT 17702-41-9, Decaborane(14) 28377-97-1 32124-79-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxy steroid)
IT **126003-44-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carborane derivative)
RN 126003-44-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 6 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:235946 HCAPLUS
DN 116:235946
ED Entered STN: 13 Jun 1992
TI Synthesis and properties of 3,17-disubstituted estrogenic steroids
AU Tong, Z. S.; Gan, G. Z.; Li, L.; Tang, Z. M.
CS Inst. Radiat. Med., Acad. Mil. Med. Sci., Beijing, 100850, Peop. Rep. China
SO Yaoxue Xuebao (**1992**), 27(3), 236-40
CODEN: YHHPAL; ISSN: 0513-4870
DT Journal
LA Chinese
CC 32-3 (Steroids)
Section cross-reference(s): 8
GI



AB Ten title radioprotective estrogens, e.g., I [R = H, Me, cyclopentyl; X = NOMe, N(CH2)nCH2OH, n = 1, 2], II (R1 = H, Me, CH2CH2OH) and III were prepared I [R = cyclopentyl, X = N(CH2)nCH2OH, N = 1, 2] showed better protective effect in mice than estradiol upon 750 rad γ-irradiation with

60Co. Several compds. increased 30-day survival rate by 35-80% in mice exposed to 900 rad of irradiation when administered i.p. 0.1 mg per mouse 24 h before irradiation

ST estratrienol prepn radioprotectant

IT Radioprotectants
(estratrienols, against γ-rays)

IT **141318-37-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)

IT **14982-15-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

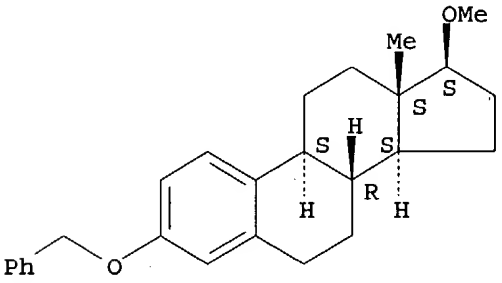
IT 2774-51-8P **4954-12-5P** 6038-28-4P 27543-03-9P 94514-10-0P 94514-11-1P 94514-13-3P 94514-15-5P 94876-43-4P 97117-16-3P 141276-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and radioprotective activity of)

IT **141318-37-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)

RN 141318-37-8 HCAPLUS

CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

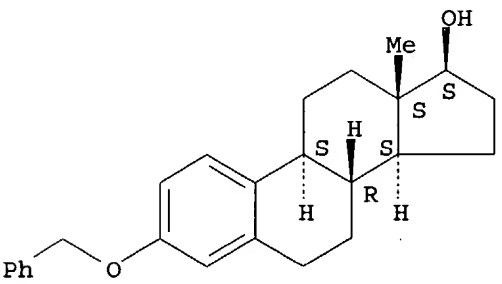


IT **14982-15-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)

RN 14982-15-1 HCAPLUS

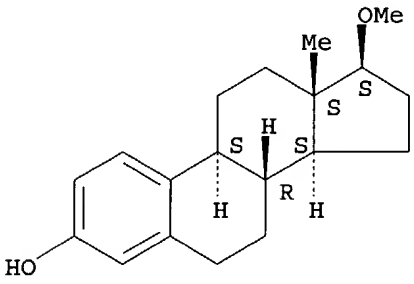
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **4954-12-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and radioprotective activity of)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



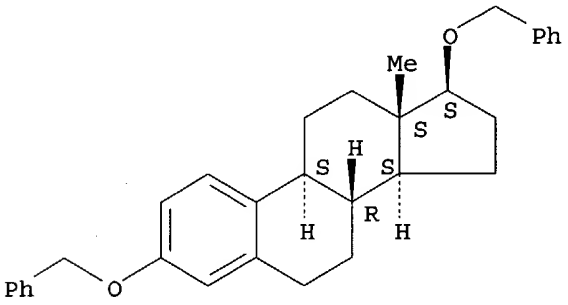
L59 ANSWER 7 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:246452 HCAPLUS
DN 114:246452
ED Entered STN: 28 Jun 1991
TI Aluminum trichloride-N,N-dimethylaniline: a new benzyl and allyl ether cleavage reagent
AU Akiyama, Takahiko; Hirofuji, Hajimu; Ozaki, Shoichiro
CS Fac. Eng., Ehime Univ., Matsuyama, 790, Japan
SO Tetrahedron Letters (**1991**), 32(10), 1321-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 114:246452
AB Benzyl and allyl ethers were cleaved readily on treatment with AlCl3 and N,N-dimethylaniline to give parent alcs. in high yields. Comparisons of N,N-dimethylaniline and anisole are also described.
ST ether allyl benzyl cleavage; aluminum chloride dimethylaniline ether cleavage
IT Bond cleavage
(of benzyl and allyl ethers, by aluminum trichloride-dimethylaniline)
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(allyl, ether cleavage of, by aluminum trichloride-dimethylaniline)
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzyl, ether cleavage of, by aluminum trichloride-dimethylaniline)
IT 121-69-7, N,N-Dimethylaniline, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(ether cleavage by aluminum trichloride and, of benzyl and allyl ethers)
IT 7446-70-0, Aluminum trichloride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(ether cleavage by dimethylaniline and, of benzyl and allyl ethers)
IT 6793-92-6, Benzyl p-bromophenyl ether 7278-60-6 64740-44-9
69455-04-5 70770-06-8, Benzyl 3-phenylpropyl ether 75364-26-0
93981-51-2 96124-85-5 101747-16-4 104330-36-1 133992-66-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(ether cleavage of, by aluminum trichloride-dimethylaniline)
IT 50-28-2P, Estra-1,3,5(10)-triene-3,17-diol (17β)-, preparation
57-88-5P, Cholest-5-en-3-ol (3β)-, preparation 106-41-2P,

p-Bromophenol 122-97-4P, 3-Phenylpropanol 3360-41-6P, 4-Phenylbutanol 6946-99-2P 17608-41-2P 24536-40-1P **55561-42-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by ether cleavage)

IT **69455-04-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ether cleavage of, by aluminum trichloride-dimethylaniline)

RN 69455-04-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

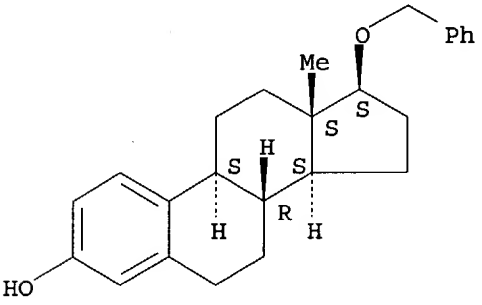
Absolute stereochemistry.



IT **55561-42-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by ether cleavage)

RN 55561-42-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 8 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:429367 HCAPLUS
DN 113:29367
ED Entered STN: 21 Jul 1990
TI HPLC determination of steroidal impurities in mestranol and ethynylestradiol
AU Levchenko, N. K.; Osokin, D. M.; Torgov, I. V.; Tuguntaev, G. I.; Sokolova, T. M.; Arzamastsev, A. P.
CS Inst. Bioorg. Khim. im. Shemyakina, Moscow, USSR
SO Khimiko-Farmatsevticheskii Zhurnal (**1990**), 24(3), 84-6
CODEN: KHFZAN; ISSN: 0023-1134
DT Journal
LA Russian
CC 64-2 (Pharmaceutical Analysis)

AB After TLC separation on a Silufol UV254 plate and identification by using 10% phosphormolybdenic acid in EtOH, steroidal microimpurities were determined in ethynylestradiol and mestranol by HPLC using different columns, mobile phases comprising EtOAc-CHCl3, MeHO-CHCl3, and CHCl3-petroleum ether, and UV spectrophotometric detection at 254 nm. The method is suitable for the quality control of these drugs.

ST ethynylestradiol mestranol impurity detn HPLC; chromatog liq ethynylestradiol mestranol impurity; steroid impurity ethynylestradiol mestranol HPLC

IT Steroids, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurities in ethynylestradiol and mestranol, by HPLC)

IT Pharmaceutical analysis
(steroidal impurities determination in ethynylestradiol and mestranol by HPLC
in)

IT Chromatography, column and liquid
(high-performance, steroidal impurities determination in ethynylestradiol and
mestranol by)

IT 50-28-2, Estradiol, analysis 53-16-7, Estrone, analysis
1035-77-4, 3-Methylestradiol 1624-62-0, 3-Methylestrone
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurity in ethynylestradiol and mestranol, by HPLC)

IT 7627-90-9 33526-46-4, 17β-Methoxyethynylestradiol
119309-39-6, 17α-Isobutylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurity in ethynylestradiol, by HPLC)

IT 7548-45-0, 3,17-Dimethoxyethynylestradiol 7627-94-3
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurity in mestranol, by HPLC)

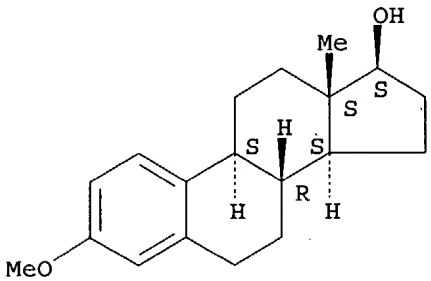
IT 57-63-6 72-33-3, Mestranol
RL: ANST (Analytical study)
(steroidal impurities determination in, by HPLC)

IT **1035-77-4**, 3-Methylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurity in ethynylestradiol and mestranol, by HPLC)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

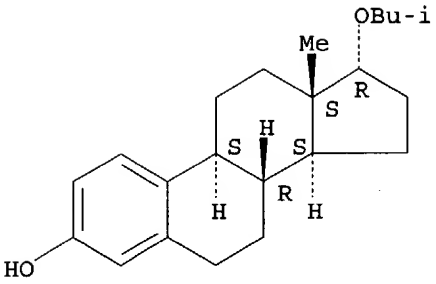


IT **119309-39-6**, 17α-Isobutylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as impurity in ethynylestradiol, by HPLC)

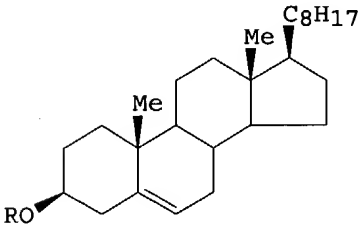
RN 119309-39-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 9 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:158724 HCAPLUS
DN 112:158724
ED Entered STN: 28 Apr 1990
TI Steroids. Part CCCXLIII. Synthesis of 2-propynyl ethers of steroid alcohols
AU Pouzar, Vladimir; Schneiderova, Lenka; Drasar, Pavel; Strouf, Oldrich; Havel, Miroslav
CS Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 166 10/6, Czech.
SO Collection of Czechoslovak Chemical Communications (**1989**), 54(7), 1888-902
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
CC 32-7 (Steroids)
OS CASREACT 112:158724
GI

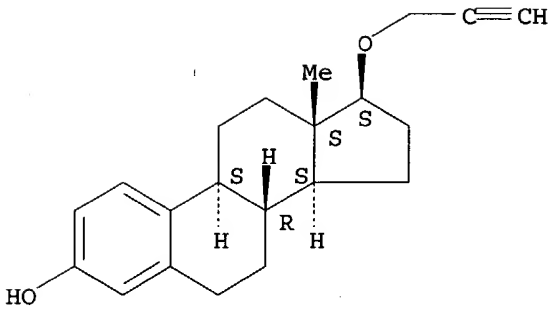


I

AB Title ethers were prepared by treating the appropriate hydroxy steroid with CH.tplbond.CCH2Br under conditions of phase-transfer catalysis. Thus, cholesterol (I, R = H) was treated with CH.tplbond.CCH2Br under various phase-transfer conditions to give ether I (R = CH2C.tplbond.CH).
ST propynyl ether steroid alc
IT Etherification
(of hydroxy steroids with propargyl bromide under phase-transfer conditions)
IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(propynyloxy, preparation of, from propargyl bromide under phase-transfer conditions)
IT 126003-46-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(Oppenauer oxidation of)
IT 105644-82-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(detosylation-epimerization of)
IT 107-30-2

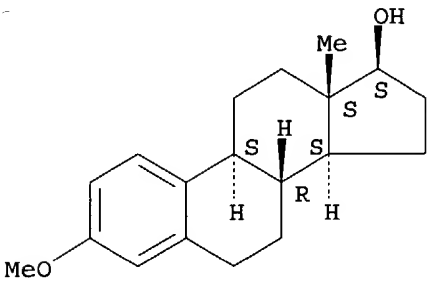
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification by, of androstenediol acetate)
IT 106-96-7, Propargyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification by, of hydroxy steroids under phase-transfer conditions)
IT 1639-43-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with chloromethyl Me ether)
IT 53-43-0 57-88-5, Cholesterol, reactions 145-13-1 66168-96-5 88128-34-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with propargyl bromide under phase-transfer conditions)
IT 58-22-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of,, with propargyl bromide under phase-transfer conditions)
IT 126003-45-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Oppenauer oxidation of)
IT 126003-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
IT 126003-33-6P 126003-36-9P 126003-39-2P 126003-43-8P 126003-47-2P 126024-80-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)
IT 41781-86-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, with propargyl bromide)
IT 5419-51-2P 126003-32-5P 126003-38-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of, with propargyl bromide under phase-transfer conditions)
IT 4975-52-4P 18000-76-5P 126003-29-0P 126003-30-3P 126003-34-7P 126003-35-8P 126003-37-0P 126003-40-5P 126003-41-6P 126003-42-7P **126003-44-9P** 126003-48-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 110-87-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-protection by, of hydroxysteroids)
IT 53-16-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(O-protection of, with dihydropyran)
IT **126003-44-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 126003-44-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



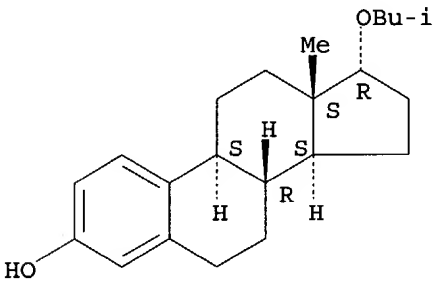
L59 ANSWER 10 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:121535 HCAPLUS
DN 110:121535
ED Entered STN: 03 Apr 1989
TI High-performance liquid chromatographic analysis of the by-products of the synthesis of ethynylestradiol, mestranol, 17α-hydroxyprogesterone caproate and 17α-hydroxy-6-dehydroprogesterone acetate
AU Levchenko, N. K.; Osokin, D. M.; Torgov, I. V.; Arzamastsev, A. P.; Sokolova, T. M.; Tuguntaev, G. I.
CS M. M. Shemyakin Inst. Bioorg. Chem., Moscow, 117871, USSR
SO Journal of Chromatography (**1988**), 456(2), 427-30
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
CC 64-3 (Pharmaceutical Analysis)
AB Impurities in the samples and mother liquors of title compds. were separated by preparative HPLC on a Prep Pak silica column with a refractiometric detector. The compds. were identified by spectral methods and determined by anal. HPLC and TLC. Some of the impurities were estrone, estradiol and estrone Me ethers, 17α-isobutylestradiol.
ST ethynylestradiol impurity detn HPLC; mestranol impurity detn HPLC; hydroxyprogesterone caproate impurity detn HPLC; hydroxy dehydroprogesterone acetate impurity detn HPLC; progesterone ester impurity detn HPLC; HPLC steroid impurity detn; chromatog steroid impurity detn
IT Steroids, analysis
RL: ANST (Analytical study)
(determination of impurities in, by HPLC)
IT Chromatography, column and liquid
(high-performance, of impurities in steroidal drugs)
IT 50-28-2, Estradiol, analysis 53-16-7, Estrone, analysis **1035-77-4**, Estradiol 3-methyl ether 1624-62-0, Estrone 3-methyl ether 33526-46-4, Ethynylestradiol 17-methyl ether **119309-39-6**, 17α-Isobutylestradiol 119309-40-9, 16-Methoxyethynylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in ethynylestradiol by HPLC)
IT 57-63-6, Ethynylestradiol 72-33-3, Mestranol 425-51-4, 17α-Hydroxy-6-dehydroprogesterone acetate 630-56-8, 17α-Hydroxyprogesterone caproate
RL: AMX (Analytical matrix); ANST (Analytical study)
(impurities determination in, by HPLC)
IT **1035-77-4**, Estradiol 3-methyl ether **119309-39-6**, 17α-Isobutylestradiol
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in ethynylestradiol by HPLC)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 119309-39-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

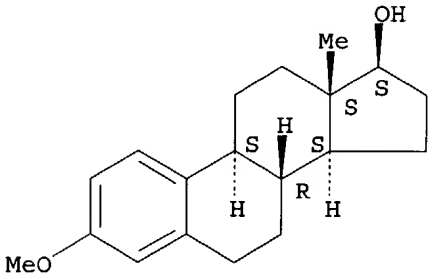


L59 ANSWER 11 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:62244 HCAPLUS
DN 104:62244
ED Entered STN: 08 Mar 1986
TI Steroid binding to the cytosolic estrogen receptor from rat uterus. Influence of the orientation of substituents in the 17-position of the 8β- and 8α-series
AU Kaspar, Peter; Witzel, Herbert
CS Inst. Biochem., Univ. Muenster, Muenster, D-4400, Fed. Rep. Ger.
SO Journal of Steroid Biochemistry (**1985**), 23(3), 259-65
CODEN: JSTBBK; ISSN: 0022-4731
DT Journal
LA English
CC 2-2 (Mammalian Hormones)
Section cross-reference(s): 32
AB The exact chemical and sterical requirements in the 17-position of 8β- and 8α-estrogens for an effective binding to the cytosolic receptor of immature rat uterus were investigated by competition expts. under non-equilibrium conditions. O or N functions with free electron pairs seem to be of essential importance in the 17-position. In contrast to 17α-methyl-, -vinyl-, or -ethynyl-substituents, a 17α-Et group strongly disturbs receptor binding. Also, the introduction of a quasi equatorial allene or a 17β-ethynyl group reduces receptor binding. In comparison to the 8β-estrogens, the 8α-derivs. always showed lower, but still significant receptor binding and similar response to changes of substituents in the 17-position.
ST estrogen receptor steroid binding structure
IT Steroids, biological studies
RL: BIOL (Biological study)

(estrogen receptor binding of, mol. structure in relation to)
IT Uterus, composition
(estrogen receptors of, steroids binding by, mol. structure in relation to)
IT Receptors
RL: BIOL (Biological study)
(for estrogen, of uterus, steroids binding by, mol. structure in relation to)
IT Estrogens
RL: BIOL (Biological study)
(receptors for, of uterus, steroids binding by, mol. structure in relation to)
IT Cytoplasm
(cytosol, estrogen receptor of, of uterus, steroids binding by, mol. structure in relation to)
IT Molecular structure-biological activity relationship
(estrogen receptor-binding, of steroids)
IT 53-16-7, biological studies 517-06-6, biological studies
RL: BIOL (Biological study)
(decomposition and estrogen receptor binding of, mol. structure in relation to)
IT **1035-77-4** 1743-60-8 2553-34-6 20989-33-7 89471-74-9
89471-79-4 89497-41-6 89576-56-7 99898-94-9 99946-38-0
RL: PROC (Process)
(estrogen receptor binding of, mol. structure in relation to)
IT 50-28-2, biological studies 53-63-4 57-91-0 302-76-1
517-04-4
RL: BIOL (Biological study)
(estrogen receptor of uterus cytosol binding of, mol. structure in relation to)
IT **99899-00-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)
IT 57-63-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)
IT 7628-02-6P 20989-33-7P 99898-92-7P 99898-95-0P 99946-34-6P
99946-35-7P 99946-36-8P 99946-37-9P 99946-39-1P **100017-39-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogen receptor binding of, mol. structure in relation to)
IT 57-63-6P 57-91-0P 4717-38-8P 7678-95-7P 15384-74-4P 99946-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogen receptor of uterus cytosol binding of, mol. structure in relation to)
IT 99946-40-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 99898-93-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and isomerization of, estrogen receptor binding and mol. structure in relation to)
IT 99898-99-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 4245-41-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and its reaction with methanesulfonic acid)

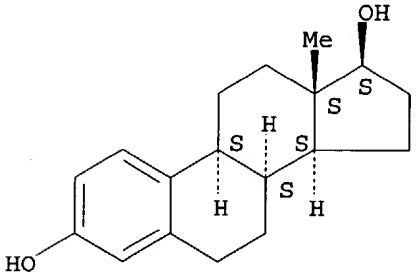
IT 99898-98-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and its reaction with nitroperbenzoic acid)
IT 99898-97-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and reaction with potassium acetate and methanesulfonic acid and hydrolysis of)
IT 5982-51-4
RL: BIOL (Biological study)
(reduction and estrogen receptor binding of, mol. structure in relation to)
IT **1035-77-4**
RL: PROC (Process)
(estrogen receptor binding of, mol. structure in relation to)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



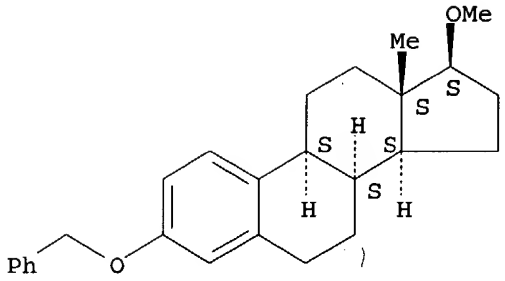
IT **517-04-4**
RL: BIOL (Biological study)
(estrogen receptor of uterus cytosol binding of, mol. structure in relation to)
RN 517-04-4 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (8α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



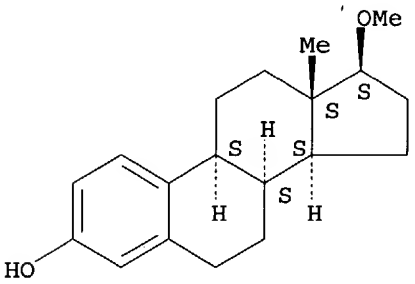
IT **99899-00-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)
RN 99899-00-0 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (8α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **100017-39-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogen receptor binding of, mol. structure in relation to)
RN 100017-39-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (8α,17β)- (9CI) (CA INDEX NAME)

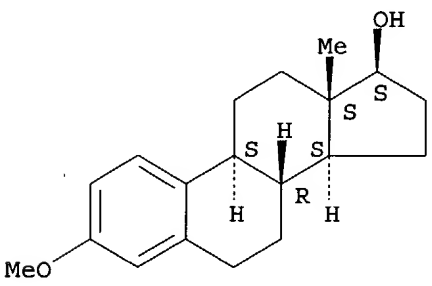
Absolute stereochemistry.



L59 ANSWER 12 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:96847 HCAPLUS
DN 100:96847
ED Entered STN: 12 May 1984
TI Specificity of an estrogen binding protein in the human vagina compared with that of estrogen receptors in different tissues from different species
AU Bergink, E. W.; Kloosterboer, H. J.; Van der Velden, W. H. M.; Van der Vies, J.; De Winter, M. S.
CS Sci. Dev. Group, Organon Int. B.V., Oss, Neth.
SO Progress in Cancer Research and Therapy (**1983**), 25(Steroids Endometrial Cancer), 77-84
CODEN: PCRTDK; ISSN: 0145-3726
DT Journal
LA English
CC 2-2 (Mammalian Hormones)
AB Estrogen-binding proteins from the myometrium, pituitary, thymus, and vagina of the rabbit; myometrium, endometrium, and vagina of the rat; and myometrium, breast tumor tissue, and MCF-7 cells of the human all displayed similar specificities with characteristics of an estrogen receptor. However, the specificity of the estrogen-binding protein in the human vagina was different from that of the human estrogen receptor; the estrogen-binding protein displayed high affinities for 17β-estradiol [50-28-2], 17α-estradiol [57-91-0], and estriol [50-27-1], but a relatively low affinity for stilbestrol [56-53-1]. Structural requirements of estrogens for binding to the estrogen receptor in the rabbit myometrium were determined and discussed.
ST estrogen binding protein vagina; receptor estrogen structure activity

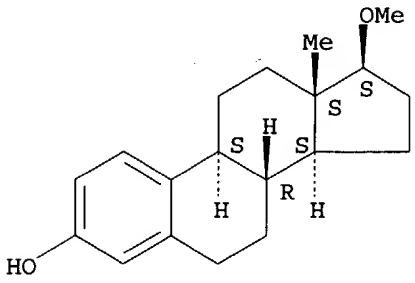
IT Receptors
RL: BIOL (Biological study)
(estrogen binding by, in human and laboratory animal, structure in relation to)
IT Neoplasm, composition
(estrogen receptor of, of mammary gland of human, specificity of)
IT Pituitary gland
Thymus gland
(estrogen receptor of, specificity of)
IT Vagina
(estrogen-binding protein of, of human and laboratory animal, specificity of)
IT Estrogens
RL: PROC (Process)
(receptor binding of, in human and laboratory animal, structure in relation to)
IT Molecular structure-biological activity relationship
(estrogen receptor-binding, of estrogens, in human and laboratory animal)
IT Proteins
RL: BIOL (Biological study)
(estrogen-binding, of vagina, of human, specificity of)
IT Uterus, composition
(myometrium, estrogen receptor of, of human and laboratory animal)
IT Mammary gland
(neoplasm, estrogen receptor of, of human, specificity of)
IT 50-27-1 50-28-2, biological studies 52-76-6 52-77-7 53-63-4
56-53-1 57-63-6 57-91-0 72-33-3 302-76-1 362-05-0 570-30-9
1035-77-4 1162-60-3 1229-24-9 1231-93-2 1464-61-5
1818-12-8 2529-54-6 2529-64-8 3398-11-6 3597-38-4 3704-15-2
4954-12-5 5444-22-4 **6544-69-0** 10448-97-2
10540-29-1 13570-81-5 13655-95-3 23637-93-6 34816-55-2
54502-78-2 54567-02-1 58212-59-2 58212-69-4 59077-04-2
66463-44-3 88899-71-2 88899-72-3 88899-73-4 88899-74-5
88899-75-6 88899-76-7 88930-00-1 88930-01-2
RL: PROC (Process)
(estrogen receptor binding of, in human and laboratory animals, structure in relation to)
IT **1035-77-4 4954-12-5 6544-69-0**
RL: PROC (Process)
(estrogen receptor binding of, in human and laboratory animals, structure in relation to)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



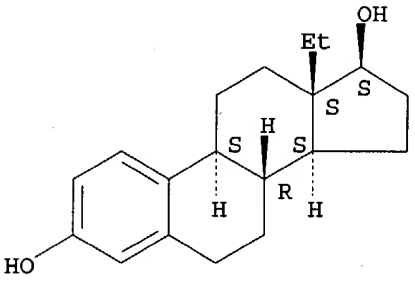
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

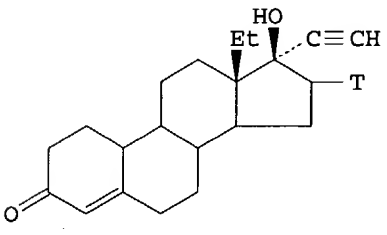


RN 6544-69-0 HCAPLUS
CN Gona-1,3,5(10)-triene-3,17-diol, 13-ethyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 13 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:22887 HCAPLUS
DN 100:22887
ED Entered STN: 12 May 1984
TI Tritium NMR spectroscopy of steroids
AU Funke, Carel W.; Kasperen, Frans M.; Wallaart, Jan; Wagenaars, Gerard N.
CS Sci. Dev. Group, Organon, Oss, 5340 BH, Neth.
SO Journal of Labelled Compounds and Radiopharmaceuticals (**1983**), 20(7), 843-53
CODEN: JLCRD4; ISSN: 0362-4803
DT Journal
LA English
CC 32-5 (Steroids)
Section cross-reference(s): 22
GI

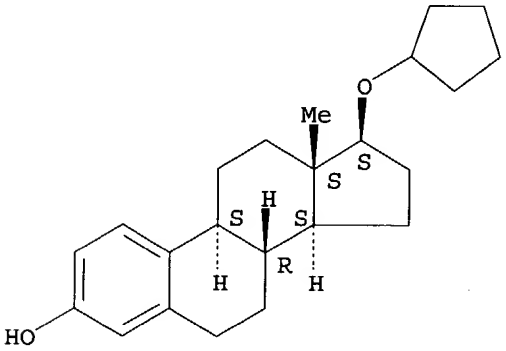


I

AB Seven tritiated pregnane-type steroids, e.g. I, were prepared and their T NMR spectra were studied; these spectra gave quant. information on the T

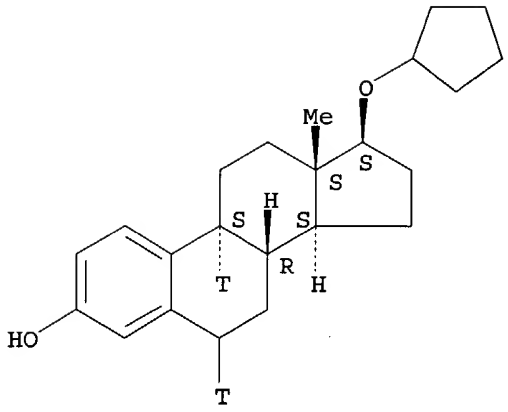
distribution in these compds.
ST tritium NMR steroid
IT Nuclear magnetic resonance
(of tritium, in pregnanes)
IT Steroids, properties
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydroxy, tritium-labeled, preparation and NMR of)
IT **85391-72-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, with tritium)
IT **88247-77-2P** 88247-78-3P 88247-79-4P 88247-80-7P
88255-64-5P 88255-65-6P 88255-66-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
IT 73991-16-9 88247-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction-tritiation of)
IT 54024-21-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(tritiation and ethynylation of)
IT 87863-63-6 88247-82-9 88247-84-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(tritiation, ethynylation, and hydrolysis of)
IT **85391-72-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, with tritium)
RN 85391-72-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **88247-77-2P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 88247-77-2 HCAPLUS
CN Estra-1,3,5(10)-trien-6,9-t2-3-ol, 17-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)

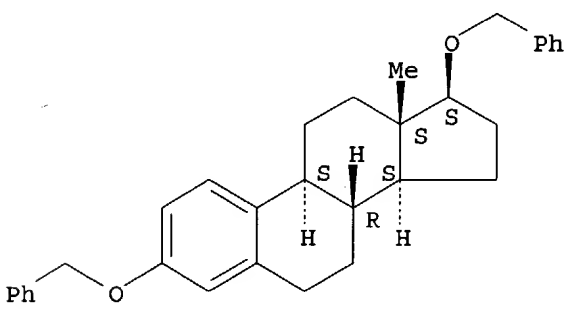
Absolute stereochemistry.



L59 ANSWER 14 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1979:202998 HCAPLUS
DN 90:202998
ED Entered STN: 12 May 1984
TI Hard acid and soft nucleophile system. New efficient method for removal of benzyl protecting group
AU Fuji, Kaoru; Ichikawa, Kohei; Node, Manabu; Fujita, Eiichi
CS Inst. Chem. Res., Kyoto Univ., Uji, Japan
SO Journal of Organic Chemistry (**1979**), 44(10), 1661-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 21-1 (General Organic Chemistry)
Section cross-reference(s): 25, 30, 32
AB Aliphatic and aromatic benzyl ethers were cleaved on treatment with a hard acid, F3B.OEt2, and a soft nucleophile, EtSH or HSCH2CH2SH, to give parent alcs. and phenols, resp. Competitive debenzylation expts. showed that the coordination of a hard acid (pulling factor) is more important than the nucleophilic attack of a soft nucleophile to the carbon atom (pushing factor) in this reaction. Thus, benzyl 2-naphthyl ether was treated with F3B.OEt2 and EtSH at room temperature for 0.8 h to give 92% 2-naphthol. Treatment of estradiol dibenzyl ether (I) with F3B.OEt2 and EtSH in CH2Cl2 at room temperature for 3 h gave 26.39% I, 11.7% estradiol 17-monobenzyl ether, 17.5% 3-monobenzyl ether, and 30.1% estradiol.
ST debenzylation benzyl ether ethanethiol; boron trifluoride debenzylation benzyl ether; nucleophile hard soft debenzylation; protecting group benzyl cleavage; estradiol benzyl ether debenzylation; naphthol benzyl ether debenzylation
IT Steroids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzyloxy, debenzylation of, by hard-soft nucleophile system)
IT Debenzylation
(of benzyl ethers by hard-soft nucleophile system)
IT Protective groups
(benzyl, removal of, by hard-soft nucleophile system)
IT Terpenes and Terpenoids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzyloxy, debenzylation of, by hard-soft nucleophile system)
IT Nucleophiles
(hard-soft, debenzylation by, of benzyl ethers)
IT 3839-48-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with (benzyloxy)bromotoluene derivative)

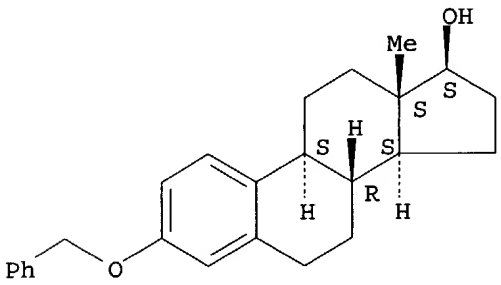
IT 2973-78-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of)
IT 613-62-7 1145-76-2 2830-53-7 5333-62-0 6793-92-6 69455-01-2
69455-02-3 69455-03-4 **69455-04-5** 69455-05-6 69455-06-7
69461-89-8 69461-90-1 69483-57-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of, by hard acid and soft nucleophile system)
IT 834-25-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(competitve debenzylation with bromophenyl benzyl ether, by hard-soft nucleophile system)
IT 75-08-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(debenzylation by, of aliphatic and aromatic benzyl ethers)
IT 69455-09-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(debenzylation of)
IT 69455-11-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)
IT 69455-12-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and bioketalization of)
IT 69455-10-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 50-28-2P, preparation 80-97-7P 89-83-8P 100-02-7P, preparation
106-41-2P 135-19-3P, preparation 6627-55-0P 13853-46-8P
13947-29-0P 69455-07-8P 69455-08-9P 69483-58-5P 69483-59-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by debenzylation of benzyl ether by hard-soft nucleophile system)
IT **14982-15-1P 55561-42-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by debenzylation of estradioldibenzyl ether with hard-soft nucleophile system)
IT 100-44-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with bromohydroxybenzaldehyde)
IT **69455-04-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylation of, by hard acid and soft nucleophile system)
RN 69455-04-5 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



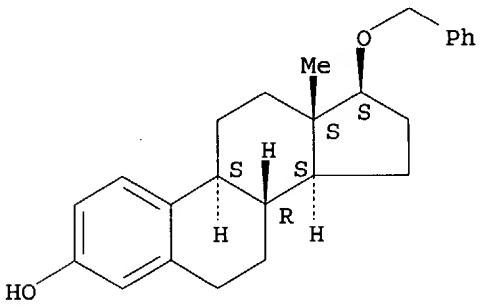
IT **14982-15-1P 55561-42-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by debenzylation of estradioldibenzyl ether with hard-soft nucleophile system)
RN 14982-15-1 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 55561-42-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 15 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:402201 HCAPLUS
DN 89:2201
ED Entered STN: 12 May 1984
TI Structural requirements for maximal inhibitory allosteric effect of estrogens and estrogen analogs on glutamate dehydrogenase
AU Pons, Michel; Michel, Francoise; Descomps, Bernard; Crastes de Paulet, Andre
CS Unite Rech. Biochim. Steroides, INSERM, Montpellier, Fr.
SO European Journal of Biochemistry (**1978**), 84(1), 257-66
CODEN: EJBCAI; ISSN: 0014-2956
DT Journal
LA English
CC 7-3 (Enzymes)
AB The inhibition of glutamate dehydrogenase by estrogens, estrogen analogs, or polyphenylethylene derivs. (.apprx.100 mols., most of them having estrogenic or antiestrogenic activities) was measured. The efficiency of these compds. in inducing allosteric inhibition of the enzyme was compared and correlated to their chemical structure: an aromatic ring A, a free phenolic group in the region of C-3 of the steroid nucleus, and a lipophilic substitution in the region of C-12, C-13, or C-17 were the main structural

features required for maximum efficiency on glutamate dehydrogenase. A tentative model for the relative orientation of the main inhibitor families is proposed. It accounts for most of the kinetic results and can be used as a tool for the selection of affinity labels directed towards the estrogen binding site of glutamate dehydrogenase.

ST glutamate dehydrogenase inhibition estrogen

IT Estrogens
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)

IT Kinetics, enzymic
(of inhibition, of glutamate dehydrogenase)

IT Molecular structure-biological activity relationship
(glutamate dehydrogenase-inhibiting, of estrogens and analogs)

IT 50-27-1 50-28-2, biological studies 53-16-7, biological studies
53-63-4 56-53-1 57-63-6 57-91-0 302-76-1 481-97-0
517-04-4 517-09-9 547-81-9 566-76-7 571-92-6
1035-77-4 1089-78-7 1213-46-3 1667-98-7 1743-60-8
1818-12-8 3398-11-6 3398-12-7 3434-88-6 3597-38-4
3736-22-9 4019-92-5 4245-41-4 **4954-12-5** 5189-40-2
5444-22-4 **5864-38-0** 5965-06-0 5976-63-6 5976-73-8
6544-69-0 10161-33-8 10218-59-4 10448-97-2 13010-22-5
13565-53-2 13864-49-8 14418-02-1 14984-42-0 14984-43-1
20796-59-2 21507-14-2 21507-16-4 21583-10-8 22831-81-8
25547-76-6 32295-36-6 33526-45-3 34816-55-2 40128-89-0
41164-28-7 **53177-70-1** 60973-93-5 61665-15-4 62013-77-8
65928-98-5 65929-00-2 66320-32-9 66422-07-9 66422-09-1
66422-11-5 66422-12-6 66422-14-8 66422-17-1 66422-18-2
66463-40-9 66463-41-0 66463-42-1 66463-43-2 66463-44-3
66463-45-4 66463-46-5 66463-47-6 66463-48-7 66463-49-8
66463-50-1 66495-43-0 **66514-24-7** 66514-25-8 66514-26-9
66514-27-0 **66537-38-0**
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)

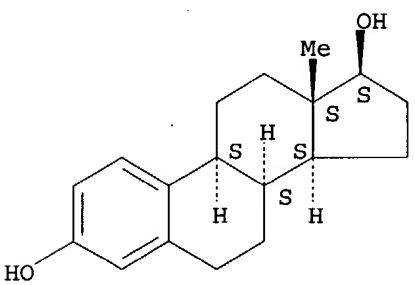
IT 9029-12-3
RL: PROC (Process)
(inhibition of, by estrogens and analogs)

IT **517-04-4 1035-77-4 3736-22-9 4954-12-5**
5864-38-0 6544-69-0 53177-70-1
66514-24-7 66537-38-0
RL: BIOL (Biological study)
(glutamate dehydrogenase inhibition by)

RN 517-04-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, (8α,17β)- (9CI) (CA INDEX NAME)

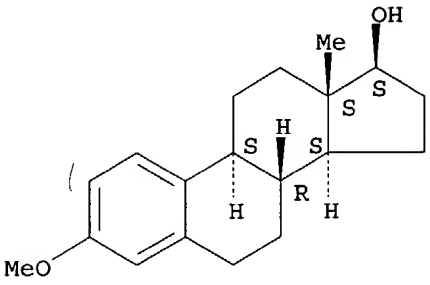
Absolute stereochemistry.



RN 1035-77-4 HCAPLUS

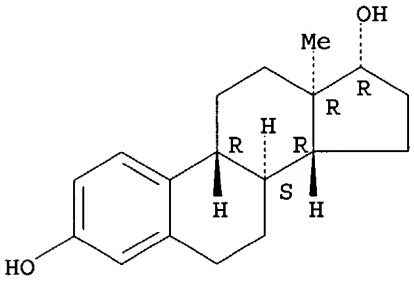
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



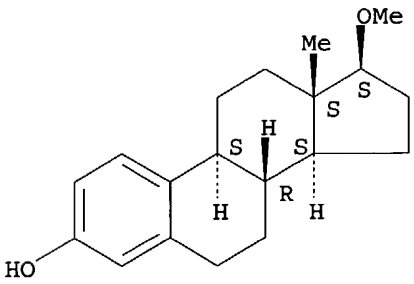
RN 3736-22-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (8α,9β,13α,14β,17.
alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



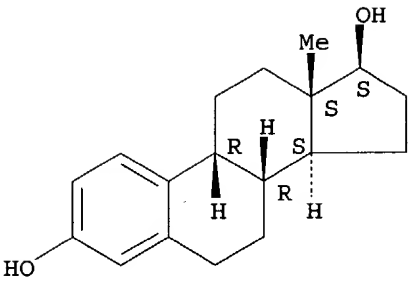
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



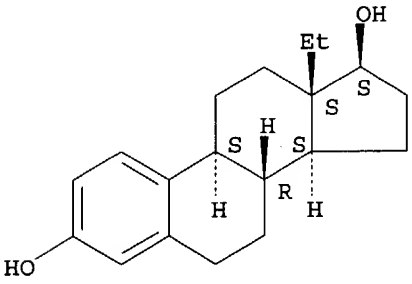
RN 5864-38-0 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (9β,17β)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.



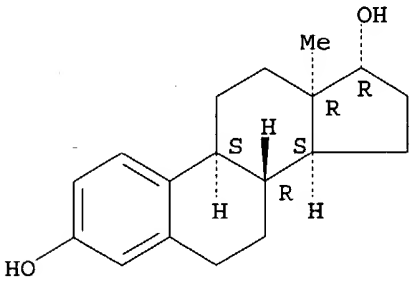
RN 6544-69-0 HCAPLUS
CN Gona-1,3,5(10)-triene-3,17-diol, 13-ethyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



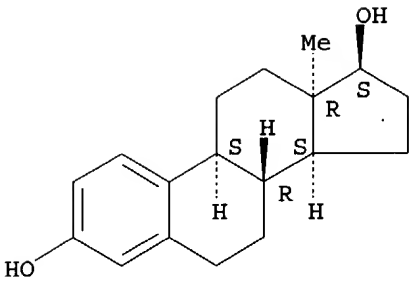
RN 53177-70-1 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (13α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



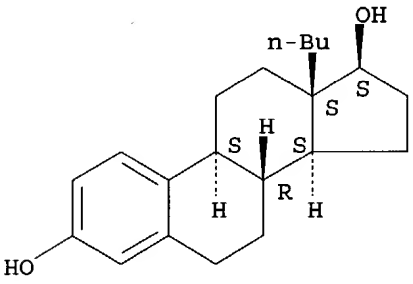
RN 66514-24-7 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (13α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 66537-38-0 HCAPLUS
CN Gona-1,3,5(10)-triene-3,17-diol, 13-butyl-, (17β)- (9CI) (CA INDEX NAME)

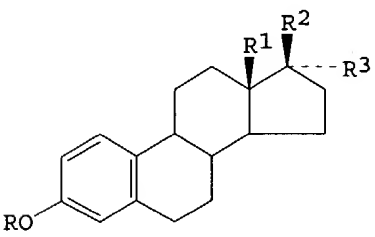
Absolute stereochemistry.



L59 ANSWER 16 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:90134 HCAPLUS
DN 86:90134
ED Entered STN: 12 May 1984
TI Esterification of phenolic hydroxyl groups in steroids
IN Schwarz, Sigfrid; Weber, Gisela
PA Ger. Dem. Rep.
SO Ger. (East), 5 pp. Addn. to Ger.(East) 114,806.
CODEN: GEXXA8
DT Patent
LA German
IC C07C167-28
CC 32-3 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DD 120016	Y	19760520	DD 1975-184239	19750217 <--
PRAI	DD 1975-184239		19750217 <--		

GI



I

AB Estratrienyl sulfonates I [R = R4SO2, (R4 = Me2CH, PhCH2, Me(CH2)7, 4-MeC6H4, cyclopentyl, cyclohexyl); R1 = H, Me, R2R3 = O, MeON; R2 = HO, MeO, Me3SiO, BuCO2, EtCO2, PhCH2CH2CO2, CH2:CHCH2O; R2 = H, HC.tplbond.C, ClC.tplbond.C, CH2:CH] (20 compds.) were prepared in 76-97% yields by treatment of I (R = H) in H2O containing an alkali hydroxide or an alkaline earth hydroxide and a quaternary ammonium salt with R4SO2Cl. Thus, I (R = R1 = H, R2 = OH, R3 = C.tplbond.CH) in H2O-NaOH containing (PhCH2)4N+Cl- was treated with Me2CHSO2Cl to give 80% I (R = Me2CHSO2, R1 = H, R2 = OH, R3 = C.tplbond.CH).

ST alkanesulfonate estratrienyl; sulfonation norpregnenynol; ethynylestradiol sulfonation; estradiol sulfonation; estrone sulfonation

IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(3β-hydroxy-17-oxygenated-1,3,5(10)-unsatd., sulfonates)

IT 28913-23-7P 28913-25-9P 29017-43-4P 29017-44-5P 29017-45-6P
32162-69-9P 38022-64-9P 38022-65-0P 42738-04-5P 42738-09-0P
42738-11-4P 54983-35-6P 55561-16-5P 55561-21-2P 55561-22-3P
55561-24-5P 55561-25-6P 55561-29-0P 55561-31-4P 61872-49-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 1939-99-7 4837-38-1 7795-95-1 10147-37-2 26394-17-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with estradienol)

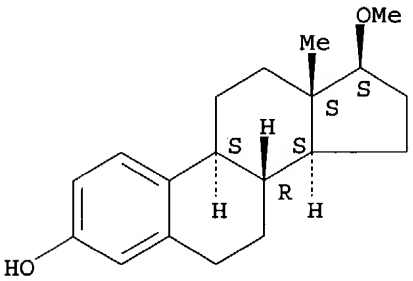
IT 50-28-2, reactions 53-16-7, reactions 57-63-6 3342-64-1 3758-34-7
4567-67-3 **4954-12-5** 7678-95-7 14012-72-7 26443-03-8
28416-77-5 33526-46-4 33760-44-0 42737-82-6 **55561-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfonylation of)

IT **4954-12-5 55561-41-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfonylation of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

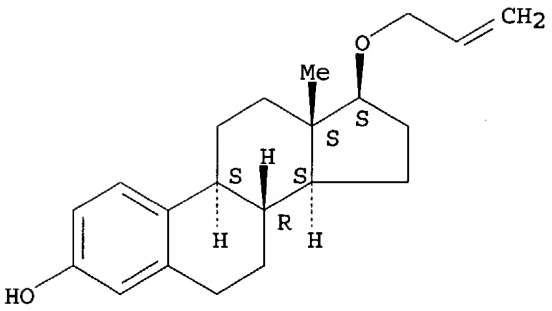
Absolute stereochemistry.



RN 55561-41-6 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17β)- (9CI) (CA INDEX NAME)

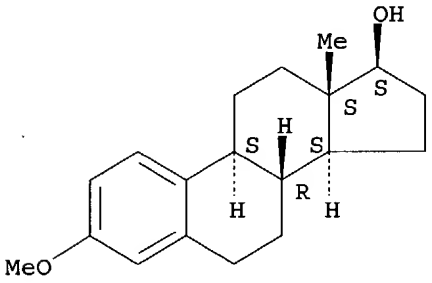
Absolute stereochemistry.



L59 ANSWER 17 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:554233 HCAPLUS
DN 85:154233
ED Entered STN: 12 May 1984
TI Study of the specificity of the estradiol-binding system of guinea pig uteri
AU Shchedrina, R. N.; Sturchak, S. V.; Bobrova, E. G.; Ishkov, V. L.; Pivnitskii, K. K.; Fanchenko, N. D.
CS All-Union Res. Inst. Obstet. Gynecol., Moscow, USSR
SO Byulleten Eksperimental'noi Biologii i Meditsiny (**1976**), 82(8), 989-93
CODEN: BEBMAE; ISSN: 0365-9615
DT Journal
LA Russian
CC 2-3 (Hormone Pharmacology)
AB The affinities of 49 steroids for the estradiol [50-28-2]-binding system of guinea pig uteri were compared. The presence of free OH groups in positions 3 (phenol) and 17β and reciprocal orientation were required for interaction with the receptor system. An intact steroid skeleton was not necessary. A polar function in ring C inhibited interaction. In addition to estradiol, 17α-ethynylestradiol [57-63-6], synestrol, and diethylstilbestrol [56-53-1] had high affinities for the estradiol-binding system.
ST estradiol receptor interaction estrane deriv
IT Uterus, metabolism
(estradiol binding by, estrane derivs. in relation to)
IT Receptors
RL: BIOL (Biological study)
(for estradiol, of uterus, estrane derivs. interaction with)
IT Estrane, derivs.
RL: BIOL (Biological study)
(estradiol binding system of uterus interaction with)
IT 50-27-1 50-50-0 53-16-7 53-45-2 53-63-4 56-53-1 57-63-6
72-33-3 84-16-2 90-15-3 113-38-2 900-83-4 963-75-7 979-32-8
1035-77-4 1089-78-7 1125-78-6 1217-09-0 1624-62-0
1630-83-7 **1852-96-6** 2299-08-3 2529-64-8 2639-53-4
3736-22-9 6218-29-7 14550-57-3 15833-07-5 19590-55-7
32436-64-9 32436-65-0 32436-66-1 34124-99-7 **38781-59-8**
39662-38-9 40481-16-1 54064-57-2 54064-60-7 54064-61-8
58395-78-1 60779-03-5 60779-04-6 60779-05-7 60779-06-8
60788-62-7 60812-06-8 60827-74-9 60872-64-2
RL: BIOL (Biological study)
(estradiol binding system of uterus interaction with)
IT 50-28-2, biological studies
RL: BIOL (Biological study)
(uterus binding of)
IT **1035-77-4 1852-96-6 3736-22-9**
38781-59-8

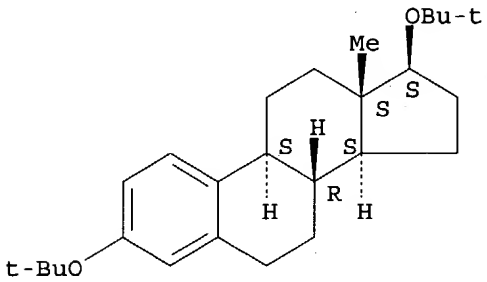
RL: BIOL (Biological study)
(estradiol binding system of uterus interaction with)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



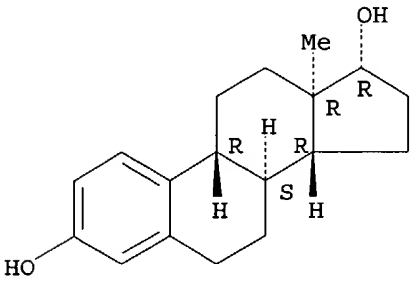
RN 1852-96-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



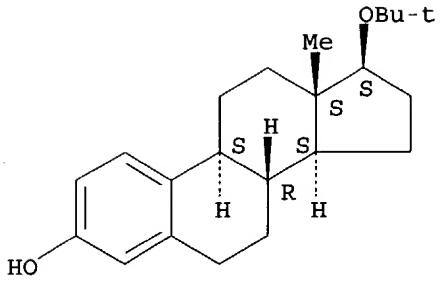
RN 3736-22-9 HCAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, (8α,9β,13α,14β,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 18 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:125520 HCAPLUS
DN 82:125520
ED Entered STN: 12 May 1984
TI Steroids. 15. Sulfonyloxy derivatives of estrogens
AU Schwarz, S.; Weber, G.; Schreiber, M.
CS Wiss. Lab., VEB Jenapharm, Jena, Ger. Dem. Rep.
SO Pharmazie (**1975**), 30(1), 17-21
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
CC 32-5 (Steroids)
GI For diagram(s), see printed CA Issue.
AB Estranes I (R = alkyl, cycloalkyl, CH2Ph, aminoalkyl; R1 = C.tplbond.CH, C.tplbond.CCl, CH:CH2, Et, H; R2 = OH, OSiMe3, alkoxy, acyloxy; R1R2 = O, NOH, NOSiMe3, NOAc, NOMe) (66 compds.) were prepared, e.g. by treating the 3-hydroxyestranes with RSO2Cl.
ST estrane sulfonyloxy; sulfonate estrane; norpregnatrienyl alkanesulfonate; estradiol alkanesulfonate; ethynylestradiol alkanesulfonate
IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(3-hydroxy-1,3,5(10)-unsatd., sulfonated)
IT 41781-86-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of)
IT 57-63-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
IT 1689-02-7 1828-66-6 10147-37-2 10539-95-4 13360-57-1 20588-68-5 26394-17-2 35856-62-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of 17-(trimethylsiloxy)-19-nor-17α-pregna-1,3,5(10)-trien-20-yn-3-ol by)
IT 10147-37-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of norpregnatrienynediol)
IT 28416-77-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, with sulfonyl chlorides)
IT **4954-12-5P 55561-41-6P 55561-42-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
IT 55561-43-8P 55561-44-9P 55561-45-0P 55561-46-1P 55561-47-2P 55561-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and etherification of)
IT 55561-38-1P 55561-39-2P 55561-40-5P 55561-49-4P 55561-50-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 3381-23-5P 28913-31-7P 28913-32-8P 28913-34-0P 28913-44-2P
29017-43-4P 29017-44-5P 42738-04-5P 42738-09-0P 42738-11-4P
52310-88-0P 52310-89-1P 52310-90-4P 54983-32-3P 54983-33-4P
55561-09-6P 55561-10-9P 55561-11-0P 55561-12-1P 55561-13-2P
55561-14-3P 55561-16-5P 55612-89-0P 55786-15-7P 55786-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

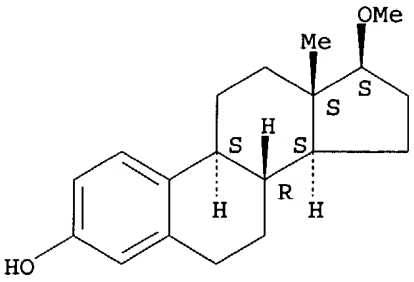
IT 4236-42-4P 28913-23-7P 28913-35-1P 28913-36-2P 54983-34-5P
54983-35-6P 54983-36-7P 54983-37-8P 54983-38-9P 55561-15-4P
55561-17-6P 55561-18-7P 55561-19-8P 55561-20-1P 55561-21-2P
55561-23-4P 55561-24-5P 55561-25-6P 55561-26-7P 55561-27-8P
55561-28-9P 55561-29-0P 55561-30-3P 55561-31-4P 55561-32-5P
55561-33-6P 55561-34-7P 55561-35-8P 55561-36-9P 55561-37-0P
55561-51-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 55561-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, esterification, and etherification of)

IT **4954-12-5P 55561-41-6P 55561-42-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

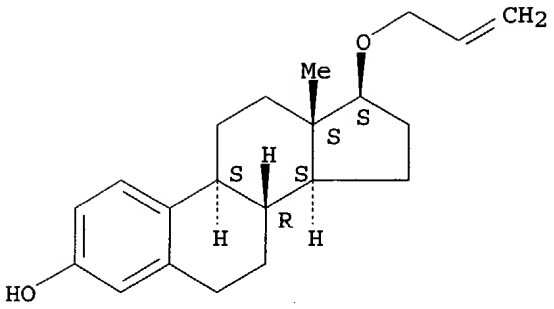
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



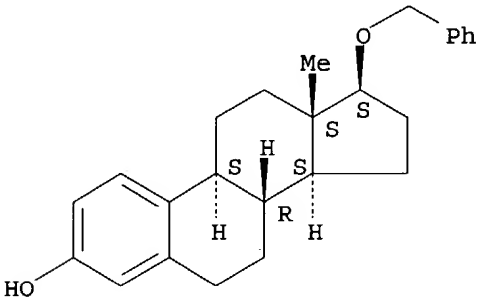
RN 55561-41-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 55561-42-7 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)

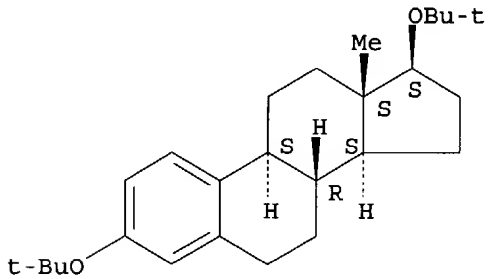
Absolute stereochemistry.



L59 ANSWER 19 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:121187 HCAPLUS
DN 80:121187
ED Entered STN: 12 May 1984
TI Replacing the phenol hydroxy group with hydrogen. Reductive cleavage of alkyl esters of estrogens by lithium in ethers
AU Cherkasov, A. N.; Golubovskaya, L. E.; Pivnitskii, K. K.
CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR
SO Zhurnal Organicheskoi Khimii (**1974**), 10(2), 320-8
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 32-3 (Steroids)
GI For diagram(s), see printed CA Issue.
AB The estratrienol ether I (R = Me3CO) was refluxed in an Ar atmospheric in glyme containing Li to give I (R = HO). Under the same conditions I (R = MeOCH2O, tetrahydro-2H-pyran-2-yloxy) yielded I (R = H), and I (R = MeO, Me2CHO) gave a mixture of I (R = H, HO). Analogous cleavage products were obtained from estradiol and estrone ethers.
ST estratrienol ether cleavage; alkoxyestratriene ether cleavage
IT Steroids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(3-alkoxy-1,3,5(10)-unsatd., reductive cleavage of)
IT 50-28-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of)
IT 53-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(ketalization and etherification of)

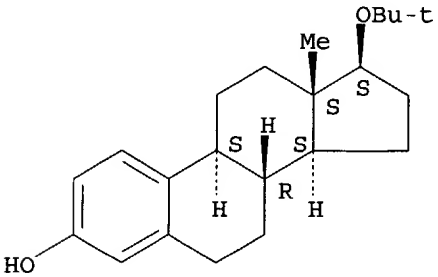
IT 38781-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 75-26-3 107-30-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with estratrienol)
IT 53-63-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isopropylbromide)
IT **1852-96-6** 3589-91-1 38781-54-3 **38781-59-8**
52509-95-2 52509-96-3 52509-97-4 52610-62-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive cleavage of)
IT 115-11-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with estratrienol)
IT **1852-96-6 38781-59-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive cleavage of)
RN 1852-96-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17β)- (9CI)
(CA INDEX NAME)

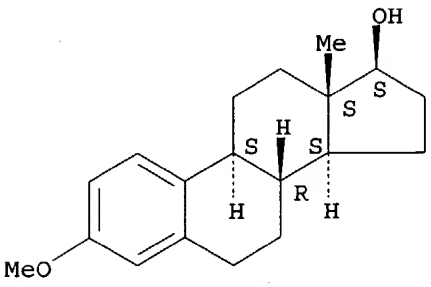
Absolute stereochemistry.



L59 ANSWER 20 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:533109 HCAPLUS
DN 79:133109
ED Entered STN: 12 May 1984
TI Comparative study of estrogen action
AU Raynaud, Jean P.; Bouton, Marie M.; Gallet-Bourquin, Danielle; Philibert, Daniel; Tournemine, Colette; Azadian-Boulanger, Genevieve

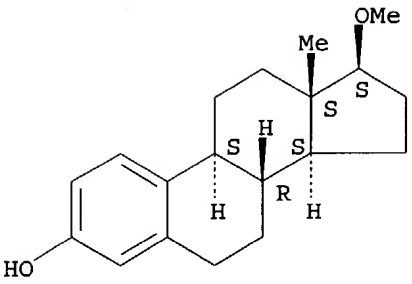
CS Cent. Rech., Roussel-Uclaf, Romainville, Fr.
SO Molecular Pharmacology (**1973**), 9(4), 520-33
CODEN: MOPMA3; ISSN: 0026-895X
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
AB The tissue distribution, metabolism, uterine uptake, and plasma and tissue binding of 8estradiol (I) [50-28-2] and 8ethynylestradiol (II) [57-63-6] derivs. were studied in rats in vivo and in vitro, and the results were related to uterotropic activity. Introduction of a methoxy group in position 11 of II, and especially I, increased uterotropic activity, whereas methylation of OH groups in postions 3 and 17 decreased it. Uterotropic activity was directly related to binding of the compds. by the 8 S uterine cytosol receptor in vivo. Activity could not be related to binding in vitro. Binding to plasma was not a prerequisite for activity but could modulate it.
ST estradiol deriv uterotropic; ethynylestradiol deriv uterotropic; uterotropic estradiol deriv
IT Cytoplasm
(estradiol derivs. binding by, of uterus, uterotropic activity of in relation to)
IT Blood plasma
(estradiol derivs. metabolism by, uterotropic activity in relation to)
IT Uterus, metabolism
(of estradiol derivs., uterotropic activity in relation to)
IT Molecular structure-biological activity relationship
(uterotropic, of estradiol derivs.)
IT 50-28-2, biological studies 57-63-6 72-33-3 **1035-77-4** **4954-12-5** **4954-14-7** 7548-45-0 21507-14-2 21507-16-4 21507-17-5 33526-45-3 33526-46-4 33526-47-5 33526-48-6 33713-12-1 34816-55-2
RL: BIOL (Biological study)
(uterotropic activity of)
IT **1035-77-4** **4954-12-5** **4954-14-7**
RL: BIOL (Biological study)
(uterotropic activity of)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



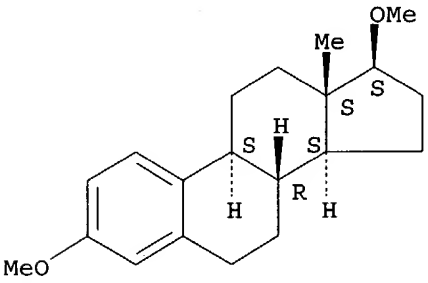
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-14-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 21 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:427594 HCAPLUS
DN 79:27594
ED Entered STN: 12 May 1984
TI Specificity of the estrogen receptor of human uterus
AU Haehnel, Roland; Twaddle, Ella; Ratajczak, Thomas
CS Dep. Obstet. Gynaecol., King Edward Mem. Hosp., Subiaco, Australia
SO Journal of Steroid Biochemistry (**1973**), 4(1), 21-31
CODEN: JSTBBK; ISSN: 0022-4731
DT Journal
LA English
CC 2-3 (Hormone Pharmacology)
AB The estrogen receptor specificity of the human uterus was determined from the relative abilities of various steroids to compete with 17β-estradiol (I) [50-28-2] for receptor sites in the uterine cytosol fraction. Highest affinity for the receptor required a free phenolic OH group on C3 and an alc. group having the β-configuration at C17, the former being particularly critical Me groups at C1 or C4 decreased the affinity drastically, whereas the effect of a Me group at C2 was relatively slight. Addnl. O functions in ring D, addnl. substituents on ring A, and unsatn. in ring B decreased the affinity for the receptor, while the presence or absence of the angular Me group at C13 had no influence.
ST steroid uterus estrogen receptor
IT Molecular structure-biological activity relationship
(estrogen receptor affinity-affecting, of steroids)
IT Uterus
(estrogen receptors of, specificity of)
IT Receptors
RL: BIOL (Biological study)
(for estrogen, of uterus, specificity of)
IT 50-23-7 50-27-1 53-16-7 53-43-0 53-45-2 53-63-4 56-53-1

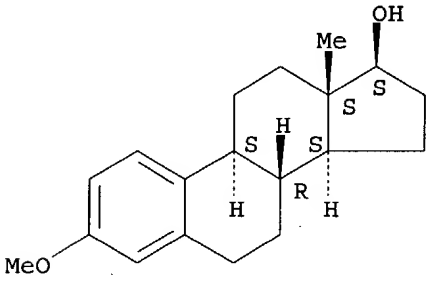
57-63-6 57-83-0, biological studies 57-91-0 58-22-0 68-96-2
145-13-1 434-22-0 474-86-2 481-95-8 481-96-9 481-97-0 517-09-9
547-81-9 566-75-6 571-20-0 793-89-5 **1035-77-4** 1090-04-6
1150-90-9 1156-92-9 1217-09-0 1228-72-4 1229-33-0 1474-53-9
1624-62-0 1806-98-0 1818-12-8 1818-13-9 1818-29-7 1852-50-2
1852-53-5 2259-89-4 2479-91-6 2529-64-8 3232-69-7 3233-69-0
3434-88-6 3597-38-4 **4954-12-5** 5635-50-7 15093-14-8
15270-30-1 20431-33-8 20592-42-1 35577-54-9 35577-55-0
42028-17-1 42028-18-2 42028-20-6 42028-21-7
RL: BIOL (Biological study)
(estradiol binding by uterus in response to)

IT 50-28-2, biological studies
RL: BIOL (Biological study)
(receptors for, of uterus, specificity of)

IT **1035-77-4 4954-12-5**
RL: BIOL (Biological study)
(estradiol binding by uterus in response to)

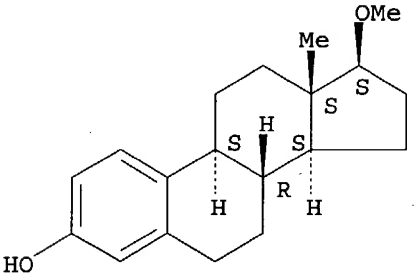
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

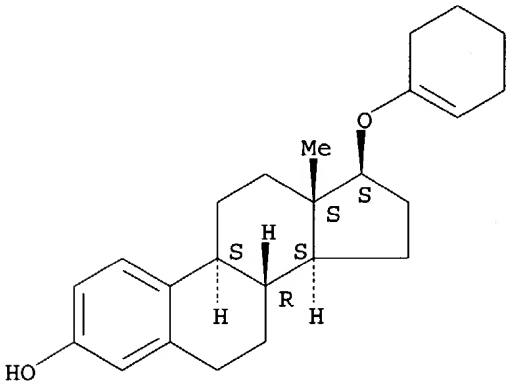


L59 ANSWER 22 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:106316 HCAPLUS
DN 78:106316
ED Entered STN: 12 May 1984
TI 1,3,5(10)-Estratrien-17β-yl enol ethers and acetals. New classes of orally and parenterally active estrogenic derivatives
AU Gardi, Rinaldo; Vitali, Romano; Falconi, Giovanni; Ercoli, Alberto
CS Warner Vistor Steroid Res. Inst., Casatenovo, Italy
SO Journal of Medicinal Chemistry (**1973**), 16(2), 123-7

CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 2-5 (Hormone Pharmacology)
OS CASREACT 78:106316
AB A number of labile 17-ethers of estradiol showed uterotrophic activity greater than that of estradiol, and in some cases comparable to that of ethynylestradiol. Especially active orally at 0.3-0.9 nmole/day in mice were cycloalkenyl ethers with 5-9-membered rings, such as 17β-(cyclopent-1-enyloxy)estra-1,3,5(10)-trien-3-ol propionate (I) [13885-28-4], and mixed ketals such as 17β-[(1-methoxycyclopentyl)oxy]estra-1,3,5(10)-trien-3-ol (II) [13885-25-1]. High and long-lasting parenteral uterotrophic activity in rats was shown after single s.c. doses of 0.05 μmole of cycloalkenyl ethers with 8-15-membered rings such as 17β-(cyclooct-1-enyloxy)estra-1,3,5(10)-trien-3-ol m-chlorobenzoate [28275-58-3]. The depot activity of these compds. may result from their high lipophilicity and from slow cleavage of the ether linkage to release estradiol. The enol ethers were prepared from the parent 17β-hydroxyestratrienes by acid-catalyzed exchange etherification with alkyl enol ethers or acetals of the appropriate aldehyde or ketone. The acetal and ketal derivs. were prepared by acid-catalyzed addition of the 17β-hydroxy steroid to suitable Me or Et enol ethers.
ST estradiol enol ether estrogen; uterotrophic estradiol enol ether
IT Estrogenic hormones
RL: BIOL (Biological study)
(estratrienyl acetals and enol ethers)
IT Uterus
(estratrienyl acetals and enol ethers effect on)
IT Molecular structure-biological activity relationship
(estrogenic, of estratrienyl acetals and enol ethers)
IT 53-16-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
IT 3000-64-4P 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P
13885-29-5P 13885-31-9P 13885-32-0P **13885-34-2P**
13885-35-3P 13885-36-4P 13945-91-0P 13945-92-1P 21513-21-3P
28151-76-0P 28151-78-2P 28151-79-3P 28151-80-6P 28200-87-5P
28200-89-7P 28200-91-1P 28200-93-3P 28200-94-4P 28200-96-6P
28200-97-7P 28200-99-9P 28201-00-5P 28201-01-6P 28201-02-7P
28201-03-8P 28201-04-9P 28201-05-0P 28231-33-6P 28275-57-2P
28275-58-3P 28275-59-4P 28275-62-9P **41622-58-6P**
41622-59-7P **41622-60-0P** 41622-64-4P 41622-65-5P
41622-66-6P **41622-69-9P** 41622-83-7P
41622-84-8P 41622-92-8P 41622-93-9P 41622-94-0P
41622-95-1P 41622-96-2P 41622-97-3P 41622-98-4P 41622-99-5P
41623-00-1P 41623-01-2P 41623-02-3P 41623-03-4P 41623-04-5P
41623-05-6P 41623-06-7P 41623-09-0P 41623-10-3P 41623-11-4P
41623-12-5P 41623-16-9P 41623-20-5P 41623-21-6P 41680-40-4P
41787-78-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogenic activity of)
IT 28151-74-8P 28151-75-9P 28151-77-1P 28200-88-6P 28275-51-6P
28275-52-7P 28275-53-8P 28275-54-9P 28275-55-0P 28275-56-1P
41623-22-7P 41623-27-2P 41623-29-4P 41623-30-7P 41623-35-2P
41623-37-4P 41623-41-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 502-72-7 931-57-7 41623-39-6
RL: BIOL (Biological study)
(reaction with estradiol esters)
IT 957-17-5
RL: BIOL (Biological study)
(reaction with estrones)

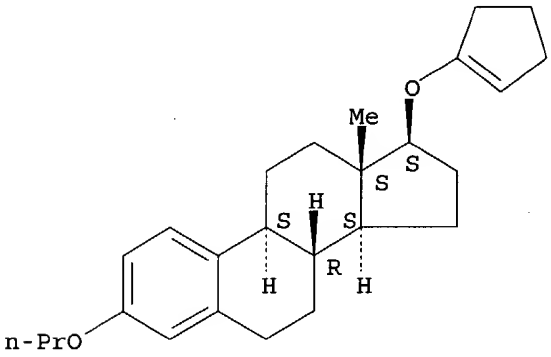
IT **13885-34-2P 41622-58-6P 41622-59-7P**
41622-60-0P 41622-66-6P 41622-69-9P
41622-84-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogenic activity of)
RN 13885-34-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



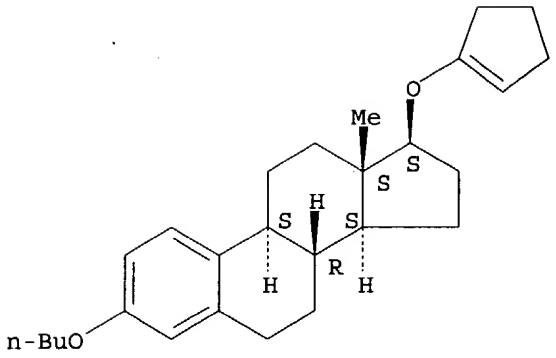
RN 41622-58-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(1-cyclopenten-1-yloxy)-3-propoxy-, (17β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



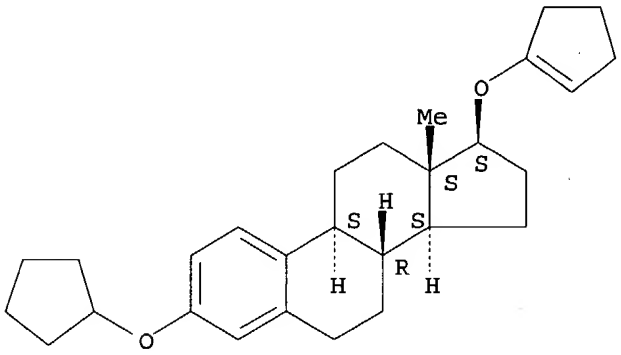
RN 41622-59-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 3-butoxy-17-(1-cyclopenten-1-yloxy)-, (17β)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



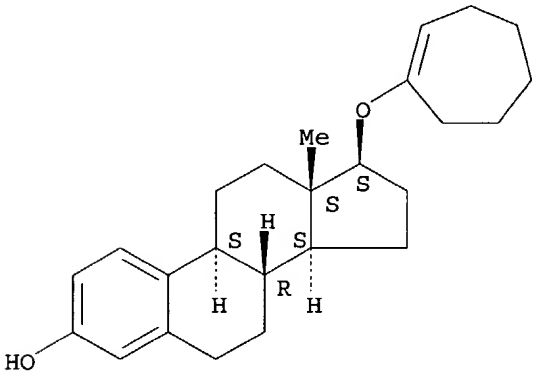
RN 41622-60-0 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(1-cyclopenten-1-yloxy)-3-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 41622-66-6 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

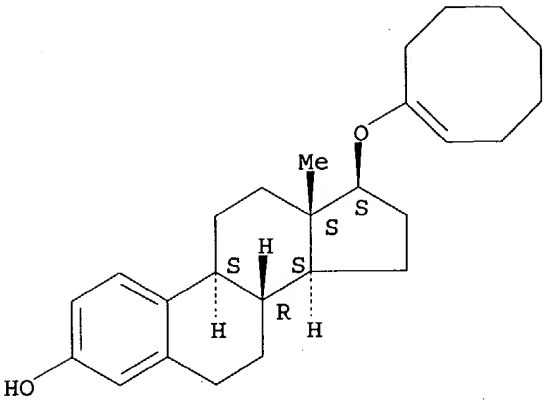
Absolute stereochemistry.



RN 41622-69-9 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cycloocten-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

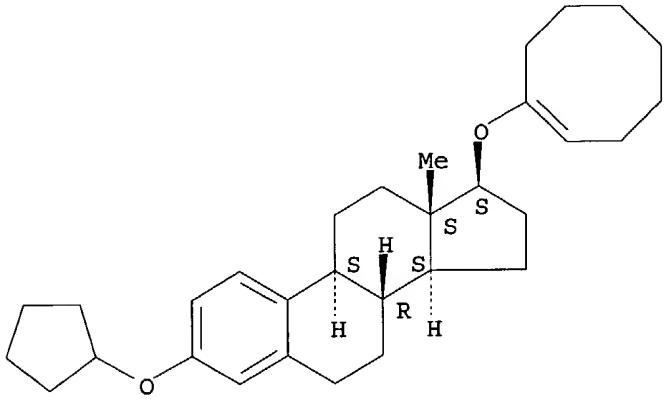
Absolute stereochemistry.

Double bond geometry unknown.



RN 41622-84-8 HCAPLUS
CN Estra-1,3,5(10)-triene, 17-(1-cycloocten-1-yloxy)-3-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)

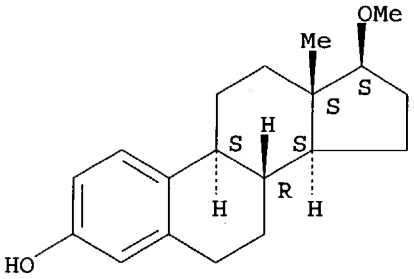
Absolute stereochemistry.
Double bond geometry unknown.



L59 ANSWER 23 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:561827 HCAPLUS
DN 77:161827
ED Entered STN: 12 May 1984
TI Degradation of steroids by intestinal bacteria. IV. Aromatization of ring A
AU Goddard, P.; Hill, M. J.
CS Bacterial. Dep., St. Mary's Hosp. Med. Sch., London, UK
SO Biochimica et Biophysica Acta (1972), 280(2), 336-42
CODEN: BBACAQ; ISSN: 0006-3002
DT Journal
LA English
CC 10-2 (Microbial Biochemistry)
AB A strain of Escherichia coli has been shown to produce estradiol from 4-androsten-3,17-dione. From the same substrate a strain of Clostridium paraputrificum produced 17-methoxy-1,3,5(10)-estratriene-3-ol.
ST Escherichia metab androstenedione; Clostridium metab androstenedione; androstenedione bacteria intestine; steroid aromatization gut bacteria
IT Escherichia coli
(estradiol formation from androstendione by)
IT Clostridium paraputrificum

(methoxyestratrienol formation from androstenedione by)
IT 63-05-8
RL: BIOL (Biological study)
(aromatization of A of, by intestinal bacteria)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
IT 50-28-2, biological studies
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Escherichia coli)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

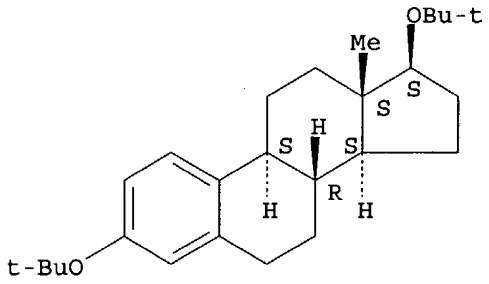
Absolute stereochemistry.



L59 ANSWER 24 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:501990 HCAPLUS
DN 77:101990
ED Entered STN: 12 May 1984
TI New method for the replacement of phenolic hydroxyl group by hydrogen. Reduction of alkoxyalkyl ethers of phenols by lithium
AU Cherkasov, A. N.; Pivnitskii, K. K.
CS Inst. Eksp. Endokrinol. Khim. Gorm., Moscow, USSR
SO Zhurnal Organicheskoi Khimii (**1972**), 8(1), 211-12
CODEN: ZORKAE; ISSN: 0514-7492
DT Journal
LA Russian
CC 32-3 (Steroids)
AB 3-(Methoxymethoxy)estrane and the tetrahydropyranyl ethers of estranol, estranediol, and estrone ethylene ketal were reduced by finely divided Li in refluxing MeOCH2CH2OMe to the corresponding 3-H compds. in 76-91% yield. The tert-Bu ethers of estranol and estranediol gave the corresponding phenols in 75-98% yields, resp., under identical conditions.
ST lithium redn steroidal phenol; alkoxyalkoxy steroid redn; dehydroxylation phenol steroidal
IT Steroids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
((alkoxyalkoxy), dealkoxylation of by lithium)
IT Dealkoxylation
(of (alkoxyalkoxy) steroids, by lithium)
IT 1217-09-0P 38781-61-2P 38781-62-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 53-63-4 **1852-96-6** 3589-91-1 14550-57-3 38781-53-2 38781-54-3 38781-56-5 38781-57-6 **38781-59-8**
RL: RCT (Reactant); RACT (Reactant or reagent)

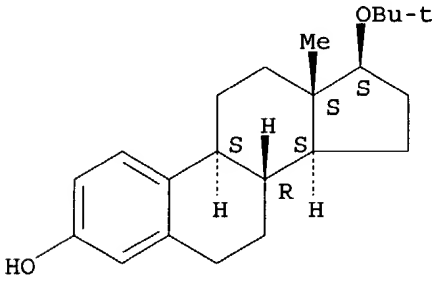
(reaction of, with lithium)
IT 7439-93-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with (alkoxyalkoxy)estrane derivs.)
IT **1852-96-6 38781-59-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with lithium)
RN 1852-96-6 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-bis(1,1-dimethylethoxy)-, (17β)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 38781-59-8 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17β)- (9CI)
(CA INDEX NAME)

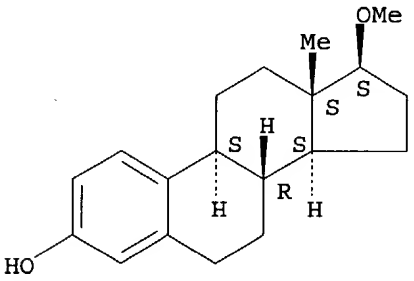
Absolute stereochemistry.



L59 ANSWER 25 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:11880 HCAPLUS
DN 76:11880
ED Entered STN: 12 May 1984
TI Aromatization of androst-4-ene-3,17-dione by human intestinal bacteria
AU Goddard, P.; Hill, M. J.
CS Dep. Bacteriol., St. Mary's Hosp. Med. Sch., London, UK
SO Biochemical Journal (**1971**), 124(5), 73P
CODEN: BIJOAK; ISSN: 0264-6021
DT Journal
LA English
CC 10 (Microbial Biochemistry)
AB Clostridium paraputrificum grown anaerobically on broth converted androst-4-ene-3,17-dione to 17β-methoxyestra-1,3,5(10)-trien-3-ol by transfer of the Me group from C-10 to the oxygen on C-17 and aromatization.
ST androstenedione metab Clostridium; steroid metab Clostridium; methoxyestratrienol synthesis Clostridium; estratrienol methoxy Clostridium; androgen aromatization bacterial

IT Clostridium paraputrificum
(methoxyestratrienol formation by, from androstenedione)
IT 63-05-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatization of, by Clostridium paraputrificum)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
IT **4954-12-5**
RL: FORM (Formation, nonpreparative)
(formation of, from androstenedione by Clostridium paraputrificum)
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

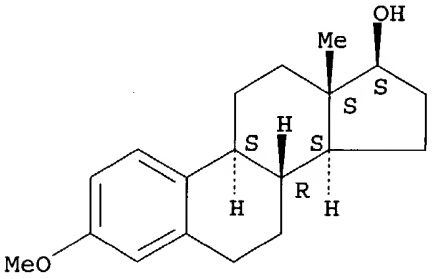
Absolute stereochemistry.



L59 ANSWER 26 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:459189 HCAPLUS
DN 75:59189
ED Entered STN: 12 May 1984
TI Pharmacodynamic model for studying the mode of action of estrogens using radioactive compounds
AU Raynaud, Jean P.; Azadian-Boulanger, Genevieve; Bourquin, Daniele; Philibert, Daniel
CS Cent. Rech. Roussel-Uclaf, Romainville, Fr.
SO Symp. Progr. Tech. Nucl. Pharmacodyn. (**1971**), Meeting Date 1970, 39-51. Editor(s): Valette, Guillaume. Publisher: Masson, Paris, Fr. CODEN: 23IDAY
DT Conference
LA French
CC 4 (Hormones and Related Substances)
AB Radioactive steroid was injected into prepubertal rats which were then sacrificed. The increased weight of the uterus as well as its incorporation of radioactivity was measured as a function of time, 0 to 70 hr, and anal. was made of estradiol, ethynyl estradiol, and 2 other derivs. The uterus reached a maximum weight at 30-40 hr. The radioactive steroids in the uterus peaked at 1-2 hr and by 10 hr were falling, while estrogen metabolites in the plasma were rising. A math. relation between the weight of the uterus and the concentration of steroid and metabolites is derived.
ST estrogen action mode; uterus wt estrogen; plasma metabolite estrogen
IT Estrogenic hormones
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, mol. structure in relation to)
IT Simulation, model
(of estrogens metabolism by uterus)
IT Uterus, metabolism
(of estrogens, model for)
IT Molecular structure-biological activity relationships

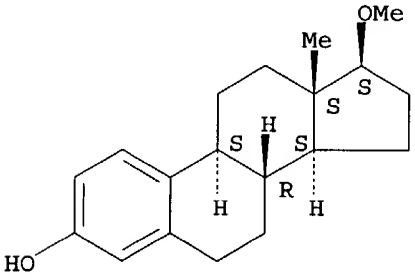
(uterus-binding, of estrogens)
IT 72-33-3 **1035-77-4 4954-12-5 4954-14-7**
7548-45-0 21507-16-4 21507-17-5 33526-45-3 33526-46-4 33526-47-5
33526-48-6 33713-12-1
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus)
IT 50-28-2, biological studies 57-63-6 21507-14-2 25918-89-2
RL: BIOL (Biological study)
(uterus binding of, estrogens effect on)
IT **1035-77-4 4954-12-5 4954-14-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



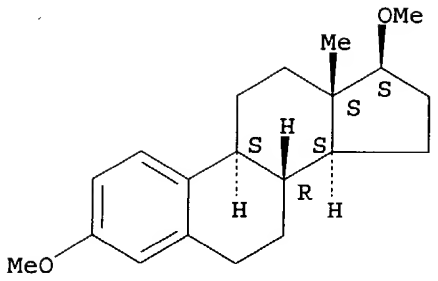
RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



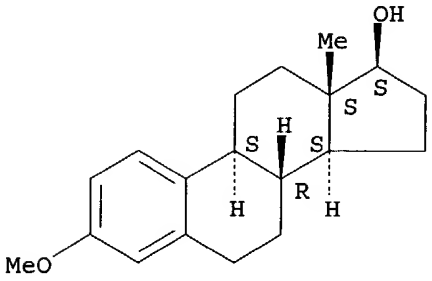
RN 4954-14-7 HCAPLUS
CN Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



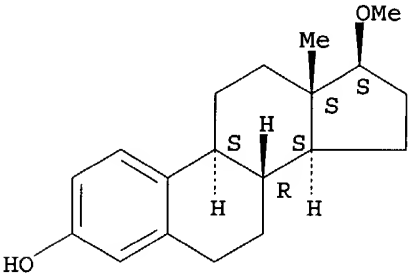
L59 ANSWER 27 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1970:432065 HCAPLUS
DN 73:32065
ED Entered STN: 12 May 1984
TI Action of natural, synthetic, and semisynthetic estrogens on deciduoma formation in rat uterus
AU Yoshino, Akio
CS Sch. Med., Jikei Univ., Tokyo, Japan
SO Tokyo Joshi Ika Daigaku Zasshi (**1969**), 84(5), 562-70
CODEN: TJIZAF; ISSN: 0040-9022
DT Journal
LA Japanese
CC 4 (Hormones and Related Substances)
AB Estrogens (I) priming action was examined with natural synthetic and semisynthetic I on deciduoma formation in rat uterus and metabolism of phospholipid, cholesterol, and nucleic acid in decidual tissue. Female rats, weighing about 160 g, were used at 3 weeks after ovariectomy. Estrone, estradiol, estriol, estrone sulfate, estrone Me ether, estradiol Me ether, estrone benzoate, estradiol benzoate, ethynyl-estradiol, diethylstilbestrol, and hexestrol were used. The natural I were effective primers for the deciduoma formation in rat uterus; synthetic I did not have this action. Natural I had more effect on phospholipid and cholesterol metabolism in rat uterus than synthetic I. Natural and synthetic I showed effects on nucleic acid metabolism.
ST estrogens deciduoma uterus; deciduoma uterus estrogens; uterus deciduoma estrogens
IT Nucleic acids
Phospholipids
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, estrogens effect on)
IT Uterus, metabolism
(of lipids and nucleic acids, estrogens effect on)
IT 50-27-1 50-28-2, biological studies 50-50-0 53-16-7, biological studies 56-53-1 57-63-6 481-97-0 **1035-77-4** 1624-62-0 2393-53-5 **4954-12-5** 5635-50-7
RL: BIOL (Biological study)
(lipid and nucleic acid metabolism by uterus in response to)
IT 57-88-5, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by uterus, estrogens effect on)
IT **1035-77-4 4954-12-5**
RL: BIOL (Biological study)
(lipid and nucleic acid metabolism by uterus in response to)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 28 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:477753 HCAPLUS
DN 71:77753
ED Entered STN: 12 May 1984
TI Mechanism of estrogen action in relation to carcinogenesis
AU Jensen, Elwood V.
CS Univ. of Chicago, Chicago, IL, USA
SO Proceedings of the Canadian Cancer Research Conference (**1966**), Volume Date 1964, 6, 143-65
CODEN: PCCRA4; ISSN: 0068-8436
DT Journal
LA English
CC 4 (Hormones)
AB cf. CA 57:6523d. When 3H-labeled estradiol (I) or 17α-methylestradiol (II) was given s.c. in saline to Sprague-Dawley rats, absorption was rapid and the level of radioactivity in the blood and nonresponsive tissues reached a maximum in 15 min., then fell rapidly, while the uterus and vagina continued to incorporate and retain radioactivity. When I or II was given s.c. in sesame oil, the levels in liver and nonresponsive tissues paralleled that in the blood, but in the uterus, vagina, anterior pituitary, and 7,12-dimethylbenz(a)anthracene - induced mammary tumors, there was a progressive uptake and retention. With hexestrol (III), retention in the vagina and uterus was more prolonged. The affinity of the uterus for estriol (IV) was not as striking as for I, but there was some retention in the growth-responsive tissues. The uterus and vagina showed no special affinity for estrone (V). Most of the uterine radioactivity after I administration was in the myometrium. The highest concentration of radioactivity was in the lamina propria with the radioactivity decreasing from the inner to outer myometrium. I was not readily taken up and retained by epithelial cells. After the

administration of 0.1 μg. I, II, or IV, all the radioactivity in the uterus and vagina was in the free steroid fraction after 15 min., 2 hrs., or 6 hrs., resp.; the same was observed in the 2 hr. uteri of III-treated animals. With V, free steroid predominated in the uterus, with some water-soluble radioactivity, but the liver and blood contained radioactivity bound to the alc.-insol. fraction and in the water-soluble form. After administration of I, II, or III, only I, II, or III appeared in the uterus and vagina, while injected IV appeared in the uterus as IV with small amts. of other polar steroids. After V administration, V was present in the uterus after 15 min. but after 2 hrs. V was gone and I was present. Metabolic transformation of I, II, and III occurred in the liver, but I, II, and III evidently stimulate growth in the rat uterus without undergoing metabolic transformation. An early if not initial step in the physiol. action of estrogenic hormones is an association with receptor sites present in the uterus, vagina, and anterior pituitary. Interaction does not involve covalent bonds but is strong enough in vivo to permit the uptake and retention of steroid against a concentration gradient. The initial association of estrogen with receptor sites was inhibited by estrogen antagonists like U-11100 and MER-25 but not actinomycin D or puromycin.

ST estrogens mechanism; mechanism estrogens; metab estrogens

IT Estrogenic hormones
RL: BIOL (Biological study)
(carcinogenesis in relation to)

IT Neoplasms, metabolism
(of estrogens in induced mammary)

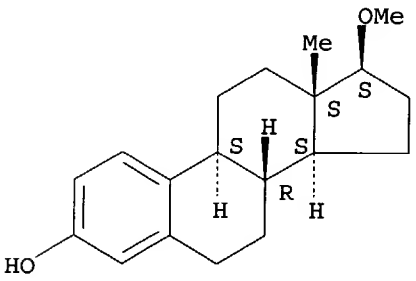
IT 50-27-1 50-28-2, biological studies **4954-12-5** 5635-50-7
RL: BIOL (Biological study)
(in reproductive tract of female after administration)

IT **4954-12-5**
RL: BIOL (Biological study)
(in reproductive tract of female after administration)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 29 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1969:68634 HCAPLUS

DN 70:68634

ED Entered STN: 12 May 1984

TI 17-Ethers of estradiol

IN Ercoli, Alberto; Gardi, Rinaldo

PA Warner-Lambert Pharmaceutical Co.

SO U.S., 5 pp.
CODEN: USXXAM

DT Patent

LA English

NCL 424243000

CC 32 (Steroids)

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3417183	A	19681217	US 1966-546506	19660502 <--
	CH 479568	A	19691015	CH 1966-479568	19660601 <--
	CH 483410	A	19691231	CH 1966-483410	19660601 <--
	DK 118462	B	19700824	DK 1966-2868	19660603 <--
	DK 121437	B	19711018	DK 1969-3171	19690612 <--
PRAI	IT 1965-12593		19650604 <--		

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are prepared by treating a 3-ester of estradiol with a functional derivative of a carbonyl compound in the presence of a catalyst. Thus, a solution of 1 g. estradiol 3-propionate (II) in 2 ml. tert-BuOH is treated with 1 ml. cyclopentanone enol methyl ether and 10 mg. p-MeC6H4SO3H to give the 17-(1-methoxycyclopentyl) (A) ether of II, m. 81-3° (MeOH-CH2Cl2), [α]2D2 44.5° (c 0.5, dioxane). Similarly is prepared the A ether of estradiol 3-acetate (III), m. 89-91°, [α]2D2 49.5° (c 0.5%, dioxane). A solution of 0.5 g. III in 25 ml. MeOH is refluxed 2 hrs. with 0.1N NaOH, the mixture concentrated, and the residue crystallized from MeOH- CH2Cl2 to give the A ether of estradiol, m. 127-9°, [α]2D2 50° (c = 0.5, dioxane). Similarly are prepared the following I [R, R1, m.p., and [α]2D2 (c 0.5, dioxane) given]: EtCO, 1-methoxycyclohexyl, -, 49°; Ac, 1-methoxycyclohexyl, 79-82°, 51.5°; H, 1-methoxycyclohexyl, 108-10°, 53.5°; EtCO, MeOC(Me)Et, 53-7°, 64°; H, MeOC(Me)Et, 109-13°, 67.5°. A mixture of 3 g. II and 5 ml. cyclopentanone diethyl acetal is heated 1 hr. at 180-200°, neutralized with a few drops pyridine, concentrated to dryness in vacuo, and crystallized from MeOH to give the 17-(cyclopent-1-enyl) ether of II, m. 91-3°, [α]2D2 61.5° (c 0.5, dioxane). Similarly are obtained the following I [R, R1, m.p., [α]2D2 (c 0.5, dioxane) given]: Ac, cyclopent-1-enyl, 126-8°, 65°; BuCO, cyclopent-1-enyl, - (oil), 53.5°; H, cyclopent-1-enyl, 73-6°, 66.5°; EtCO, cyclohex-1-enyl, 114-16°, 75°; BuCO, cyclohex-1-enyl, - (oil), 62.5°; H, cyclohex-1-enyl, 87-90°, 75.5°. I possess valuable claudogenic and estrogenic activity, especially suitable for oral use. It is advisable to stabilize the pharmaceutical compns. with alkaline substances to prevent acid hydrolysis of the 17-ethers.

ST estradiols estrogenic; estrogenic estradiols

IT 19-Norsteroids
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkoxy)

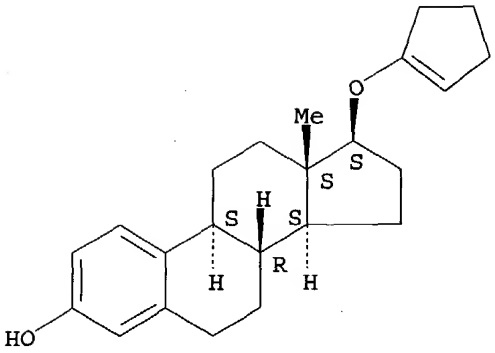
IT 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P 13885-29-5P
13885-30-8P 13885-31-9P 13885-32-0P 13885-33-1P
13885-34-2P 13885-35-3P 13885-36-4P 13885-37-5P
13945-91-0P 13945-92-1P 14258-73-2P 21513-21-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **13885-30-8P 13885-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13885-30-8 HCAPLUS

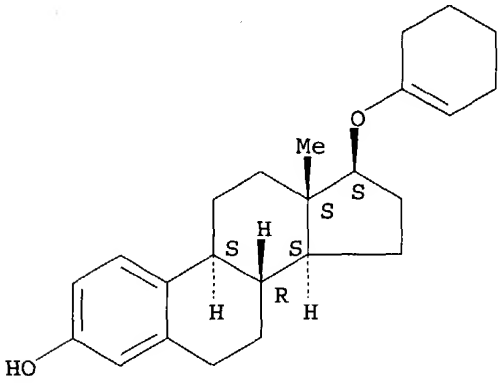
CN Estra-1,3,5(10)-trien-3-ol, 17β-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 13885-34-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 30 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:95293 HCAPLUS
DN 66:95293
ED Entered STN: 12 May 1984
TI Estradiol ethers
PA Francesco Vismara Societa per Azioni
SO Neth. Appl., 10 pp.
CODEN: NAXXAN
DT Patent
LA Dutch
IC C07C
CC 32 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	NL 6607527		19661205	NL		<--
	FR 5517			FR		
	GB 1072828			GB		
PRAI	IT		19650604	<--		

AB Estradiol 3-propionate (I) (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclopentanone enol Me ether treated about 10 min. with 10 mg. p-MeC6H4SO3H yielded the 17-(1-methoxycyclopentyl) ether (II) of I, m. 81-3° (CH2Cl2-MeOH), [α]22D 44.5° (c 0.5, dioxane). Similarly was prepared the 17-(1-methoxycyclopentyl) ether of estradiol

3-acetate (III), m. 89-91°, [α]22D 49.5° (c 0.5, dioxane). II (0.5 g.) in 25 cc. MeOH refluxed 2 hrs. with 0.1N NaOH gave the 17-(1-methoxycyclopentyl) ether of estradiol (IV), m. 127-9° [(CH2Cl)2-MeOH]. I (1 g.) in 2 cc. tert-BuOH and 1 cc. cyclohexanone enol Me ether treated with 10 mg. p-MeC6H4SO3H.C5H5N (V) gave the 17-(1-methoxycyclohexyl) ether (VI) of I. Similarly was prepared 0.95 g. 17-(1-methoxycyclohexyl) ether of III, m. 79-82°, [α]22D 51.5° (c 0.5, dioxane), from 1 g. III; its hydrolysis with 0.1N KOH gave the 17-(1-methoxycyclohexyl) ether of IV, m. 108-10°, [α]22D 53.5° (c 0.5, dioxane). I (3 g.) and 5 cc. cyclopentanone dimethyl acetal heated 1 hr. at 180-200° gave the 17-(1-cyclopentenyl) ether (VII) of I, m. 91-3° (MeOH), [α]22D 61.5° (c 0.5, dioxane). Similarly were prepared the 17-(1-cyclopentenyl) ether of III, m. 126-8°, [α]22D 65° (c 0.5, dioxane), and the oily 17-(1-cyclopentenyl) ether of estradiol 3-valerate (VIII), [α]22D 53.5° (c 0.5, dioxane) VII (1.5 g.) in 50 cc. MeOH warmed 2 hrs. with 0.5 g. K2CO3 in 5 cc. H2O yielded the 17-(1-cyclopentenyl) ether of IV, m. 73-6°, [α]22D 66.5° (c 0.5, dioxane). I (2 g.), 3 cc. cyclohexanone dimethyl acetal, 20 mg. V, and 3 cc. HCONMe2 heated 1 hr. at 180-90° gave the 17-(1-cyclohexenyl) ether (IX) of I, m. 94-6° (CH2Cl2-MeOH), [α]22D 71° (c 0.5, dioxane). Similarly were prepared the 17-(1-cyclohexenyl) ether of III, m. 114-16°, [α]22D 75° (c 0.5, dioxane), and the oily 17-(1-cyclohexenyl) ether of VIII, [α]22D 62.5° (c 0.5, dioxane). IX (2 g.) hydrolyzed with NaOH-MeOH gave the 17-(1-cyclohexenyl) ether of IV, m. 87-90°, [α]22D 75.5° (c 0.5, dioxane). EtMeC(OMNe)2 (1 g.), 30 mg. p-MeC6H4SO3H, and 5 cc. tert-BuOH with 1 g. I gave the 17-(1-methoxy-1-methylpropyl) ether of I, m. 64-8°, [α]22D 62° (c 0.5, dioxane). Similarly was prepared the 17-(1-methoxy-1-methylpropyl) ether of III, m. 53-7°, [α]22D 64° (c 0.5, dioxane), which hydrolyzed with alkali gave the 17-(1-methoxy-1-methylpropyl) ether of IV, m. 109-13°, [α]22D 67.5° (c 0.5, dioxane).

ST ESTRADIOL CYCLOPENTYL ETHERS; CYCLOPENTYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXYL ETHERS; CYCLOHEXYL ETHERS ESTRADIOL; ESTRADIOL CYCLOPENTENYL ETHERS; CYCLOPENTENYL ETHERS ESTRADIOL; ESTRADIOL CYCLOHEXENYL ETHERS; CYCLOHEXENYL ETHERS ESTRADIOL; ESTRADIOL PROPYL ETHERS

IT Steroids, preparation
RL: PREP (Preparation)
(17-alkoxy)

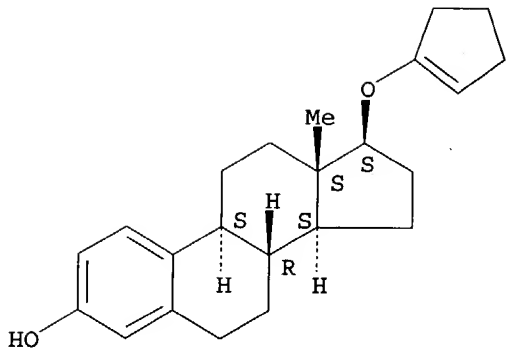
IT 13885-25-1P 13885-26-2P 13885-27-3P 13885-28-4P 13885-29-5P
13885-30-8P 13885-31-9P 13885-32-0P 13885-33-1P
13885-34-2P 13885-35-3P 13885-36-4P 13885-37-5P
13945-91-0P 13945-92-1P 14258-73-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **13885-30-8P 13885-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 13885-30-8 HCAPLUS

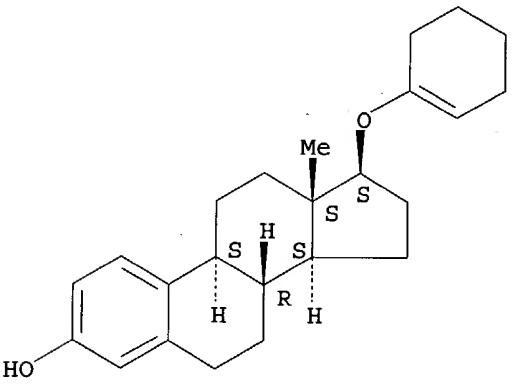
CN Estra-1,3,5(10)-trien-3-ol, 17β-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 13885-34-2 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 31 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1966:44062 HCAPLUS
DN 64:44062
OREF 64:8257f-g
ED Entered STN: 22 Apr 2001
TI 17β-Estradiol 17-methyl ether
AU Coombs, M. M.; Roderick, H. R.
CS Imp. Cancer Res. Fund, Lincoln's Inn Fields, London
SO Steroids (**1965**), 6(6), 841-4
CODEN: STEDAM; ISSN: 0039-128X
DT Journal
LA English
CC 42 (Steroids)
AB Exptl. results and characterization of various products of 17β-estradiol 17-Me ether are presented.
IT Dichroism
(circular, of 5α-estr-1(10)-en-2-one and 1,10β-dihydro derivative)
IT Nuclear magnetic resonance
(of 3,17β-dimethoxyestra-1,3,5(10)-triene)
IT Estra-1,3,5(10)-triene, 3-(2-benzoyl-4-nitrophenoxy)-2-msthoxy-
IT 1743-60-8, Estradiol, 17-acetate 4953-96-2, Estra-1,3,5(10)-trien-3-ol, 2-methoxy- **4954-12-5**, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy- 4954-13-6, Estra-1,3,5(10)-trien-3-ol,

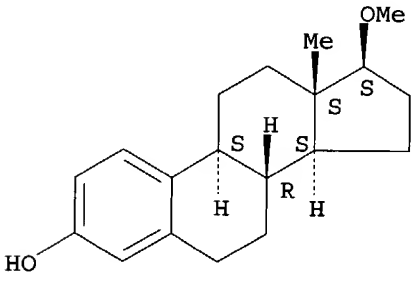
17β-methoxy-, benzoate **4954-14-7**, Estra-1,3,5(10)-triene, 3,17β-dimethoxy- 4954-16-9, Estradiol, 17-acetate, 3-p-toluenesulfonate 4954-17-0, Estradiol, 17-acetate, 3-benzoate 4967-93-5, Benzophenone, 2-(estra-1,3,5(10)-trien-3-yloxy)-5-nitro- 4967-94-6, Estra-1,3,5(10)-triene, 2-methoxy- 4967-96-8, 5α-Estr-1(10)-en-2-one 4968-11-0, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-, acetate 4999-72-8, Benzophenone, 2-[(2-methoxyestra-1,3,5(10)-trien-3-yl)oxy]-5-nitro- 5506-56-9, Benzophenone, 2-[(2-hydroxyestra-1,3,5(10)-trien-3-yl)oxy]-5-nitro- 7054-98-0, Estra-2,5(10)-diene, 2-methoxy-
(preparation of)

IT **4954-12-5**, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-
4954-14-7, Estra-1,3,5(10)-triene, 3,17β-dimethoxy-
(preparation of)

RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

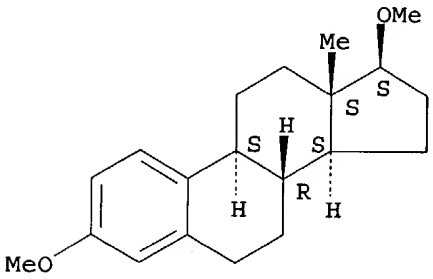
Absolute stereochemistry.



RN 4954-14-7 HCAPLUS

CN Estra-1,3,5(10)-triene, 3,17-dimethoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 32 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1964:493831 HCAPLUS

DN 61:93831

OREF 61:16379g-h

ED Entered STN: 22 Apr 2001

TI Fractionation of estrogen methyl esters and alumina column chromatography (estimation of 16-epiestriol in pregnancy urine)

AU Shida, K.; Kimura, M.; Kanbegawa, A.

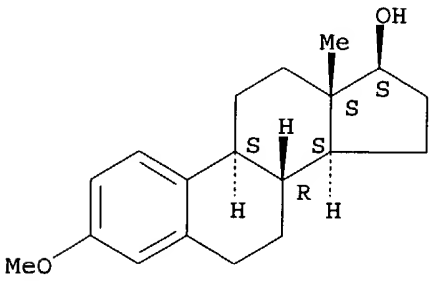
CS Med. and Dental Univ. School Med., Tokyo

SO Nippon Naibunpi Gakkai Zasshi (**1961**), 37(1), 5-9
CODEN: NNGZAZ; ISSN: 0029-0661

DT Journal

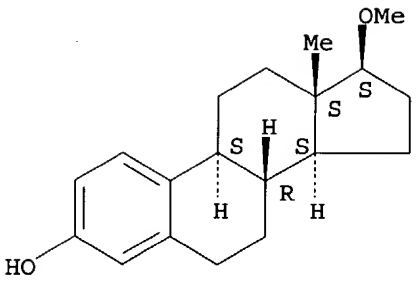
LA Unavailable
CC 58 (Hormones)
AB After boiling for 15 min. with 15% concentrated HCl, late pregnancy urine was extracted twice with ether, washed with 5% NaHCO3 and water, dried with anhydrous Na2SO4, and concd, to about 10 ml. in a water bath. The estrogens were extracted with benzene-petr. ether and reextd. with 1.6% NaOH. H3BO3 and dimethyl sulfate were added followed by stirring for 30 min. Following the addition of 30% H2O2 the methylated estrogens were chromatographed on an alumina column 0.5 + 20 cm. prepared by partial filling with petr. ether and the addition of 2.0 g. of Brockmann alumina at 18° under 10-12 mm. Hg. The Me esters of estrone, estradiol, 16-epiestriol, and estriol were eluted with 40% petr. ether in benzene, 1.0% MeOH in benzene, and 3.0% MeOH in benzene, resp. The content of 16-epiestriol reached 11.5% in late pregnancy urine. From Abstract Japan. Med. 1(15), Abstract Number 6640(1961).
IT Pregnancy
(16-epiestriol in urine in)
IT Urine
(analysis, determination of 16-epiestriol)
IT Estrogenic hormones or principles
(methyl esters, chromatography of)
IT Estra-1,3,5(10)-triene-16α,17β-diol, 3-methexy-
(determination of, in urine in pregnancy)
IT 547-81-9, Estra-1,3,5(10)-triene-3,16β,17β-triol
1035-77-4, Estra-1,3,5(10)-trien-17β-ol, 3-methoxy-
1624-62-0, Estra-1,3,5(10-trien-17-one, 3-methoxy- 3434-79-5, Estra-1,3,5(10)-triene-16β,17β-diol, 3-methoxy-
4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-
(determination of, in urine in pregnancy)
IT **1035-77-4**, Estra-1,3,5(10)-trien-17β-ol, 3-methoxy-
4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-
(determination of, in urine in pregnancy)
RN 1035-77-4 HCAPLUS
CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4954-12-5 HCAPLUS
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L59 ANSWER 33 OF 33 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:40001 HCAPLUS
DN 56:40001
OREF 56:7630a-d
ED Entered STN: 22 Apr 2001
TI Steroid derivatives. XII. Chromatography of neutral steroids on a thin aluminum oxide layer
AU Hermanek, S.; Schwarz, V.; Cekan, Z.
CS Research Inst. Nat. Drugs, Prague
SO Collection of Czechoslovak Chemical Communications (**1961**), 26, 1669-79
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA German
CC 55 (Biochemical Methods)
AB cf. CA 55, 27411c; 56, Number 5.-The use of Al2O3 without binder has the advantage of simplicity in preparing a thin layer for chromatography. Alkaline Al2O3 was used with ligroin (b. 30-50°), benzene, ligroinbenzene, and benzene-EtOH mixts. in various proportions. Δ4-3-Ketones were detected by lightly spraying with SbCl3 in CHCl3, other Δ4-substances with SbCl3 in CHCl3 with 10% SOCl2. Alkalinity of Al2O3 was without influence on Rf values and, except for formates, trichloroacetates, and trifluoroacetates, did not degrade the substances during the 10-20 min. of development. Benzene was used as the first solvent for unknown mixts. Rf values in several solvents are tabulated for some 90 steroids belonging to 3-substituted cholest-5-enes, 17-substituted 3β-acetoxyandrost-5-enes, 3βsubstituted androst-5-en-17-ones, 3β-substituted methyl-7keto-eti-5-enates, 3β-substituted cholest-5-en-7-ones, 17βsubstituted androst-4-en-3-ones, and miscellaneous classes. Chromatographic control of preparation and purity of a substance is exemplified by the separation of pregn-4-ene-17α,21-diol-3,20-dione, its diacetates, 17α,21-diacetoxypregn-5-en3β-ol-20-one, and 17α,21-diacetoxy-3β-formyloxypregn-5en-20-one and accompanying impurities. Adsorptivity of 17β-substituents increased in the following order: COOCH3, OBz, CN-COCH3, OAc, O, OH; for 3β-substituents of cholest-5-ene the order was: H, Cl, OCH3, OAc, OH, and NMe2; similarly, cyclohexylamine moved more slowly than cyclohexanol while aniline was much faster than PhOH.
IT Steroids
(separation of, on Al2O3 film)
IT Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester, acetate
Estradiol, propionate
(separation of, on Al2O3 film)
IT Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester
Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-, methyl ester, benzoate
Androst-5-ene-17β-carboxylic acid, 12α-hydroxy-17-methyl-3-oxo-

, methyl ester, p-toluenesulfonate
Cholesterol, nitrobenzoate
Pivalic acid, cholesteryl ester
(separation on Al2O3 film)

IT 57-87-4, Ergosterol 83-48-7, Stigmasterol
(chromatography of, on Al2O3)

IT 95908-73-9, Pregn-5-ene-20-carboxylic acid, 3β-hydroxy-, acetate
(chromatography on Al2O3)

IT 142-62-1, Hexanoic acid
(esters, separation on Al2O3film)

IT 53-16-7, Estrone 53-43-0, Androst-5-en-17-one, 3β-hydroxy-
57-83-0, Progesterone 57-88-5, Cholesterol 58-18-4,
Androst-4-en-3-one, 17β-hydroxy-17-methyl- 58-22-0, Testosterone
63-05-8, Androst-4-ene-3,17-dione 64-85-7, Corticosterone, deoxy-
68-96-2, Pregn-4-ene-3,20-dione, 17-hydroxy- 80-75-1,
Pregn-4-ene-3,20-dione, 11α-hydroxy- 145-13-1, Pregn-5-en-20-one,
3β-hydroxy- 152-58-9, Pregn-4-ene-3,20-dione, 17,21-dihydroxy-
302-23-8, Pregn-4-ene-3,20-dione, 17-hydroxy-, acetate 387-79-1,
Pregn-5-en-20-one, 3β,17-dihydroxy- 434-03-7, 17α-Pregn-4-en-
20-yn-3-one, 17-hydroxy- 512-04-9, Diosgenin 516-15-4,
Pregn-4-ene-3,11,20-trione 630-56-8, Pregn-4-ene-3,20-dione,
17-hydroxy-, hexanoate 640-87-9, Pregn-4-ene-3,20-dione,
17,21-dihydroxy-, 21-acetate 974-23-2, Pregn-5-en-20-one,
16α,17-epoxy-3β-hydroxy- **1035-77-4**,
Estra-1,3,5(10)-trien-17β-ol, 3-methoxy- 1061-54-7, Diosgenin,
acetate 1235-98-9, 17α-Pregna-4,20-dien-3-one, 17-hydroxy-
3604-60-2, 17α-Pregn-5-en-20-yne-3β,17-diol 4139-90-6,
Androst-5-ene-17β-carboxylic acid, 3β-hydroxy-, methyl ester,
acetate **4954-12-5**, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-
6252-45-5, Cholest-5-ene, 3β-[(tetrahydropyran-2-yl)oxy]-
14072-39-0, Pregn-5-en-20-one, 16β-bromo-3β,17-dihydroxy-
20272-84-8, Pregna-1,4-dien-20-one, 3β-hydroxy- 20867-15-6,
Pregn-5-en-20-one, 3β,17-dihydroxy-, 3-formate 31823-53-7,
Chol-5-enic acid, 3β-hydroxy-, methyl ester, acetate 71205-59-9,
Pregna-1,4-dien-20-one, 3β-hydroxy-, acetate 95557-72-5,
Pregna-1,4-dien-20-one, 3β-hydroxy-, oxime, acetate 96345-96-9,
Cholest-5-ene, 3-chloro- 107158-49-6, Cholest-5-en-3α-amine,
N,N-dimethyl-
(separation of, on Al2O3 film)

IT 50-28-2, Estradiol 56-47-3, Corticosterone, deoxy-, acetate 57-85-2,
Testosterone, propionate 126-17-0, Solasodine 521-10-8,
Androst-5-ene-3β,17β-diol, 17-methyl- 521-17-5,
Androst-5-ene-3β,17β-diol 566-28-9, Cholest-5-en-7-one,
3β-hydroxy- 570-74-1, Cholest-5-ene 601-57-0, Cholest-4-en-3-one
604-32-0, Cholesterol, benzoate 604-35-3, Cholesterol, acetate
633-34-1, Androsta-4,6-diene-3,17-dione 809-51-8, Cholest-5-en-7-one,
3β-hydroxy-, acetate 853-23-6, Androst-5-en-17-one,
3β-hydroxy-, acetate 897-06-3, Androsta-1,4-diene-3,17-dione
1045-69-8, Testosterone, acetate 1169-49-9, Testosterone, isobutyrate
1174-92-1, Cholest-5-ene, 3β-methoxy- 1175-12-8,
Androst-5-ene-3β,17β-diol, 17-benzoate 1182-65-6, Cholesterol,
p-toluenesulfonate 1255-57-8, Testosterone, p-toluenesulfonate
1259-22-9, Androst-5-ene-3β,17β-diol, 3-acetate,
17-p-toluenesulfonate 1639-43-6, Androst-5-ene-3β,17β-diol,
3-acetate 1639-44-7, Pregn-5-en-20-one, 3β-hydroxy-, benzoate
1778-02-5, Pregn-5-en-20-one, 3β-hydroxy-, acetate 1807-15-4,
Pregn-4-ene-3,20-dione, 17,21-dihydroxy-, diacetate 2080-86-6,
Androst-5-en-17-one, 3β-hydroxy-, benzoate 2088-71-3, Testosterone,
benzoate 2099-26-5, Androst-5-ene-3β,17β-diol, diacetate
4651-48-3, Stigmasterol, acetate 4860-15-5, Solasodine, diacetate
5953-63-9, Androst-5-ene-3β,17β-diol, 3-acetate, 17-benzoate
6997-41-7, Cholest-5-en-7-one, 3β-hydroxy-, benzoate 14546-23-7,
Cholest-5-en-3β-amine, N,N-dimethyl- 19637-35-5,

Androst-5-en-17-one, 3β-[(tetrahydropyran-2-yl)oxy]- 29163-23-3, Androst-5-en-17-one, 3β-hydroxy-, formate 33854-98-7, Androst-5-ene-3β,17β-diol, 17-methyl-, 3-acetate 34209-81-9, Pregn-5-en-20-one, 16α,17-epoxy-3β-hydroxy-, acetate 40768-03-4, Androst-5-ene-3β,17α-diol, 3-acetate 17-benzoate 41329-03-7, Cholesterol, pivalate 50303-03-2, Androst-5-ene-17β-carbonitrile, 3β-hydroxy-, acetate 96553-92-3, Androst-5-ene-3β,7β,17β-triol, 17-methyl-, 3,17-diacetate 96772-72-4, Cholest-5-en-7-one, 3β-hydroxy-, p-toluenesulfonate
(separation on Al2O3 film)

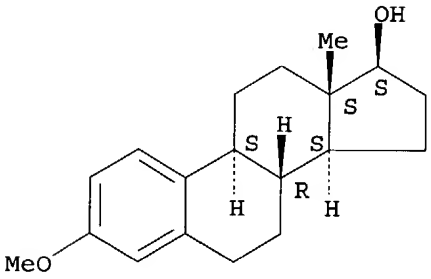
IT 1344-28-1, Aluminum oxide
(steroid separation on film of)

IT **1035-77-4**, Estra-1,3,5(10)-trien-17β-ol, 3-methoxy-
4954-12-5, Estra-1,3,5(10)-trien-3-ol, 17β-methoxy-
(separation of, on Al2O3 film)

RN 1035-77-4 HCAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 3-methoxy-, (17β)- (9CI) (CA INDEX NAME)

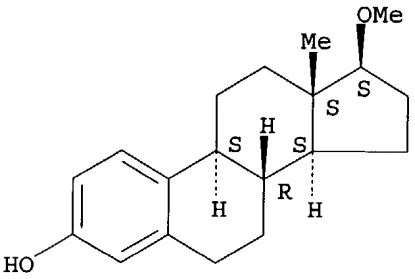
Absolute stereochemistry.



RN 4954-12-5 HCAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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(FILE 'HOME' ENTERED AT 10:33:36 ON 20 JUL 2004)
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FILE 'HCAPLUS' ENTERED AT 10:34:03 ON 20 JUL 2004

L1 1 S US20020035100/PN OR (US2001-893324# OR WO2001-US41170 OR US20
E PROKAI L/AU

L2 122 S E3,E4,E7
E SIMPKINS J/AU

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L3          245 S E3,E5,E7-E9
                SEL RN L1

     FILE 'REGISTRY' ENTERED AT 10:35:20 ON 20 JUL 2004
L4           18 S E1-E18
L5           16 S L4 AND C5-C6-C6-C6/ES
L6            9 S L5 AND 4/NR
L7            7 S L5 NOT L6
L8              STR
L9              STR L8
L10          50 S L9
L11       13381 S L9 FUL
                SAV TEMP L11 QAZI893/A
L12             STR L9
L13          22 S L12 CSS SAM SUB=L11
L14         434 S L12 CSS FUL SUB=L11
                SAV L14 QAZI893A/A
L15         119 S L14 AND NC>=2
L16          13 S L15 NOT ((MXS OR PMS OR IDS)/CI OR COMPD OR WITH OR UNSPECIFI
L17           2 S L16 NOT C18H24O2
L18          11 S L16 NOT L17
L19             STR L12
L20          23 S L19 FUL SUB=L14
                SAV L20 QAZI893B/A
L21          22 S L20 NOT 13C#
L22             STR L19
L23          99 S L22 FUL SUB=L14
                SAV L23 QAZI893C/A
L24          95 S L23 NOT L15
L25          87 S L24 NOT (T OR D)/ELS
L26          12 S L23 NOT L25
L27           9 S L26 AND C19H26O2
L28           3 S L26 AND C19H26O2 NOT (T OR D)/ELS
L29           2 S L28 NOT CYCLODEXTRIN
L30             STR L19
L31          58 S L30 FUL SUB=L14
                SAV L31 QAZI893D/A
L32          57 S L31 NOT (T OR D)/ELS
L33         169 S L5,L17,L21,L25,L29,L32
                SAV L33 QAZI893E/A
L34         168 S L33 NOT (T OR D)/ELS
L35         149 S L14 NOT L15,L34
L36          89 S L35 NOT (T OR D)/ELS
L37          46 S L36 NOT IDS/CI
L38          41 S L37 NOT (11C# OR 13C# OR 14C#)
L39          39 S L38 NOT PMS/CI

     FILE 'HCAPLUS' ENTERED AT 11:19:38 ON 20 JUL 2004
L40       52840 S L34
L41        1346 S L39
L42       53115 S L40,L41
L43          98 S L1-L3 AND L42

     FILE 'REGISTRY' ENTERED AT 11:20:19 ON 20 JUL 2004
L44           1 S 50-28-2
L45         167 S L34 NOT L44
L46          38 S L39 NOT 57-91-0

     FILE 'HCAPLUS' ENTERED AT 11:21:54 ON 20 JUL 2004
L47         605 S L45
L48         148 S L46
L49         715 S L47,L48
L50           9 S L1-L3 AND L49
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L51          706 S L49 NOT L50
L52          654 S L51 AND (PD<=20000627 OR AD<=20000627 OR PRD<=20000627)

     FILE 'REGISTRY' ENTERED AT 11:24:14 ON 20 JUL 2004
L53           33 S L45,L46 AND (C26H40O2 OR C24H36O2 OR C22H32O2)
L54            5 S L20 AND L53
L55           28 S L53 NOT L54
L56           18 S L20 NOT L54
L57           17 S L56 NOT 13C#

     FILE 'HCAPLUS' ENTERED AT 11:26:54 ON 20 JUL 2004
L58           41 S L54 OR L57
L59           33 S L58 AND L52

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:27:18 ON 20 JUL 2004
L60            5 S L54 OR L57

     FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004

     FILE 'USPATFULL, USPAT2' ENTERED AT 11:29:09 ON 20 JUL 2004

     FILE 'HCAPLUS' ENTERED AT 11:29:20 ON 20 JUL 2004

=> => fil reg
FILE 'REGISTRY' ENTERED AT 11:31:00 ON 20 JUL 2004
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STRUCTURE FILE UPDATES:   19 JUL 2004  HIGHEST RN 713066-32-1
DICTIONARY FILE UPDATES:  19 JUL 2004  HIGHEST RN 713066-32-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide can tot l21

L21  ANSWER 1 OF 22  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   623942-19-8  REGISTRY
CN   Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (8α,17β)-(±)- (9CI)
     (CA INDEX NAME)
FS   STEREOSEARCH
MF   C20 H28 O2
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT
DT.CA  CAplus document type:  Journal
RL.NP  Roles from non-patents:  PREP (Preparation); RACT (Reactant or reagent)

Relative stereochemistry.
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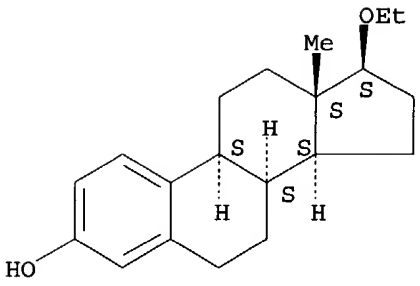


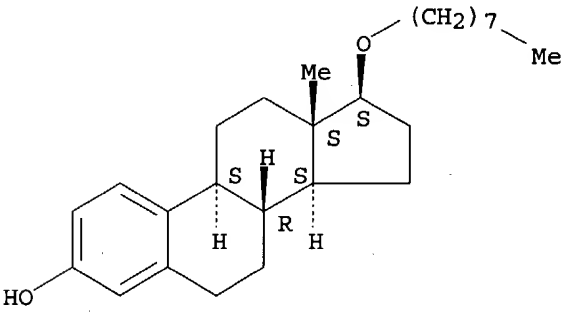
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381661

L21 ANSWER 2 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 319427-07-1 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H40 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

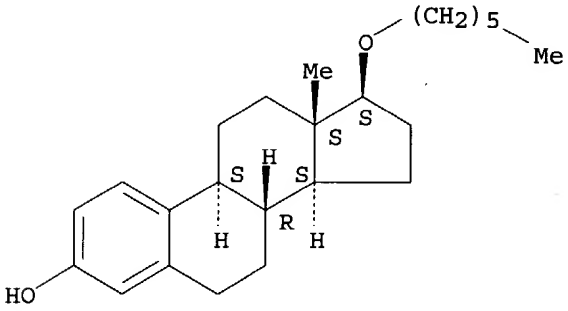
REFERENCE 2: 135:221441

REFERENCE 3: 134:101056

L21 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN

RN 319427-06-0 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(hexyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H36 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

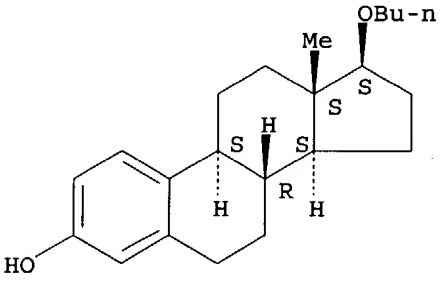
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 319427-05-9 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-butoxy-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H32 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

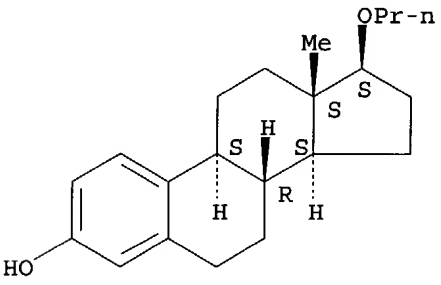
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 319427-04-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-propoxy-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H30 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

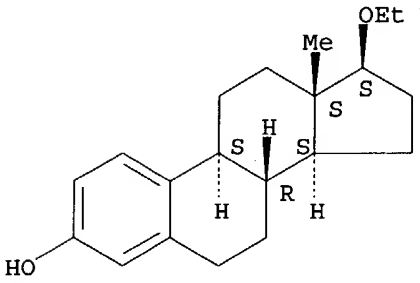
REFERENCE 1: 138:214660

REFERENCE 2: 136:85991

REFERENCE 3: 134:101056

L21 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 319427-03-7 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

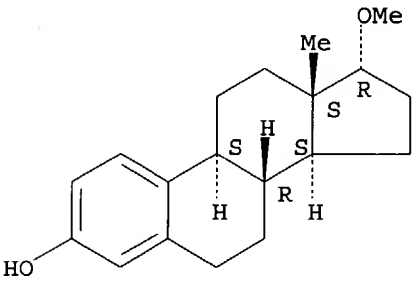
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L21 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 182823-27-4 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17α)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H26 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

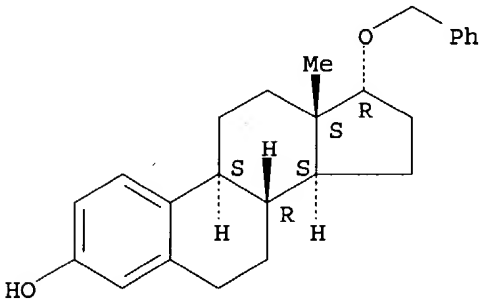
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 182624-51-7 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17α)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H30 O2

SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



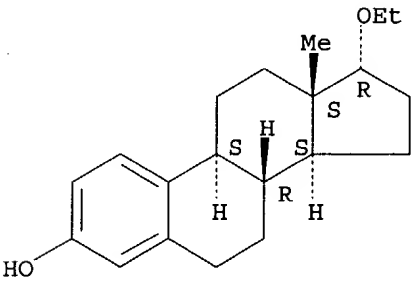
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 182624-49-3 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-ethoxy-, (17α)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

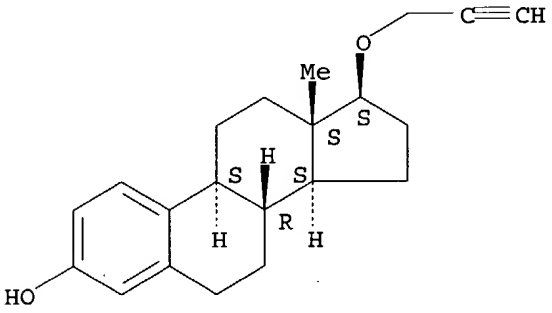
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 125:294029

L21 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 126003-44-9 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propynyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H26 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

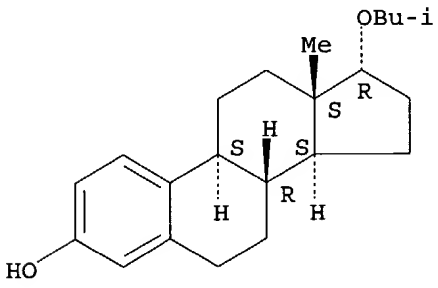
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 117:8261

REFERENCE 2: 112:158724

L21 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 119309-39-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-methylpropoxy)-, (17α)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17α-Isobutylestradiol
FS STEREOSEARCH
MF C22 H32 O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: ANST (Analytical study)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

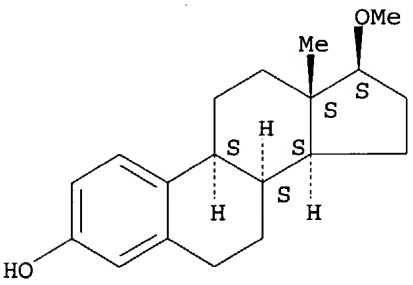
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 113:29367

REFERENCE 2: 110:121535

L21 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 100017-39-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (8α,17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H26 O2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.



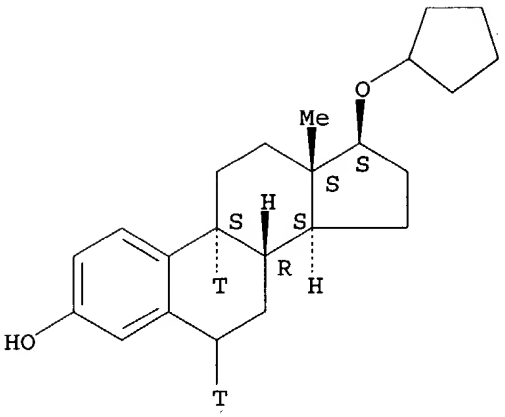
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 104:62244

L21 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 88247-77-2 REGISTRY
CN Estra-1,3,5(10)-trien-6,9-t2-3-ol, 17-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H30 O2 T2
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Absolute stereochemistry.

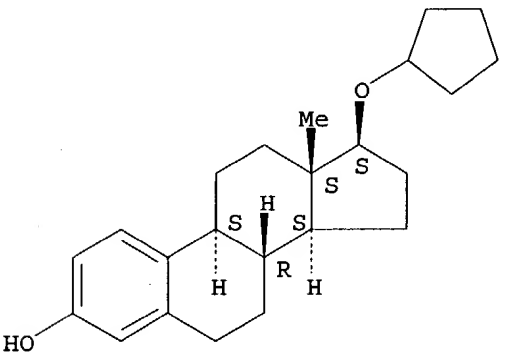


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:22887

L21 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 85391-72-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(cyclopentyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H32 O2
SR European Union (EU)
LC STN Files: CA, CAPLUS, CHEMLIST
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

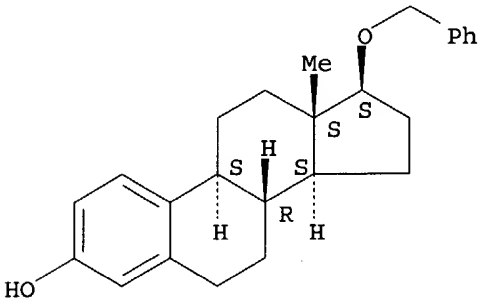
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 100:22887

L21 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55561-42-7 REGISTRY

CN Estra-1,3,5(10)-trien-3-ol, 17-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H30 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); USES (Uses)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:187955

REFERENCE 2: 138:44718

REFERENCE 3: 117:170477

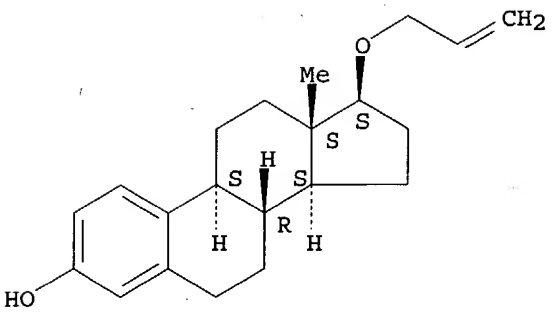
REFERENCE 4: 114:246452

REFERENCE 5: 90:202998

REFERENCE 6: 82:125520

L21 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55561-41-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(2-propenyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H28 O2
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

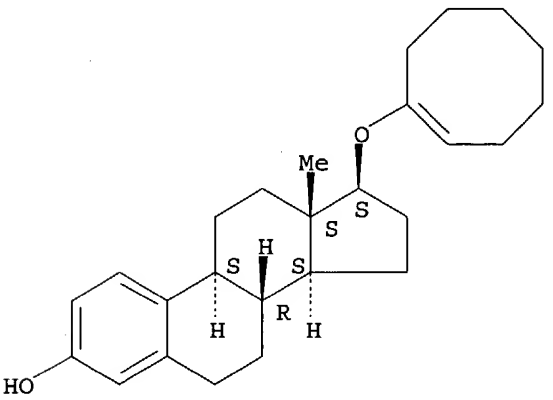
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 86:90134

REFERENCE 2: 82:125520

L21 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 41622-69-9 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cycloocten-1-yloxy)-, (17β)- (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN 17β-(Cyclooct-1'-enyloxy)estra-1,3,5(10)-trien-3-ol
FS STEREOSEARCH
MF C26 H36 O2
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.
Double bond geometry unknown.



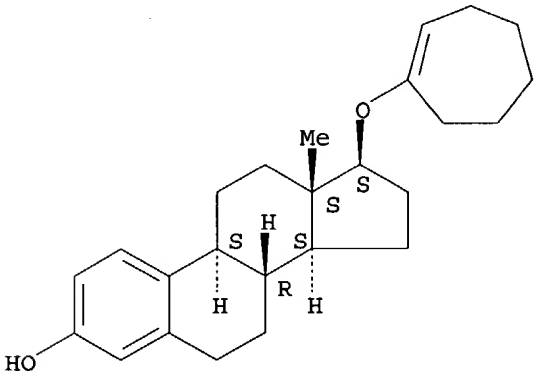
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

L21 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 41622-66-6 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohepten-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H34 O2
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.



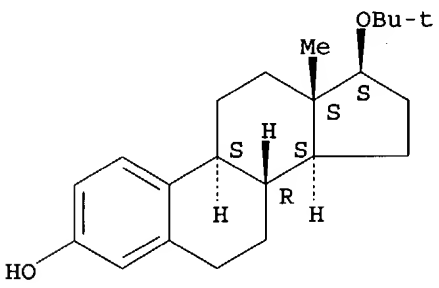
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

L21 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 38781-59-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1,1-dimethylethoxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H32 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

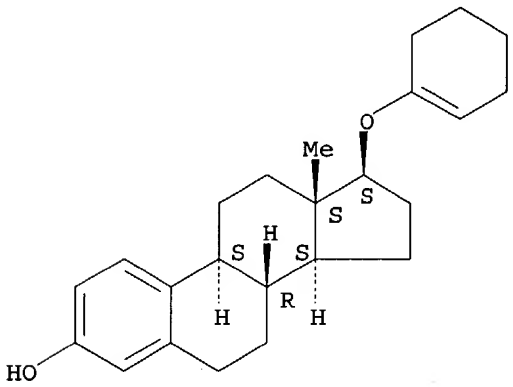
REFERENCE 1: 85:154233

REFERENCE 2: 80:121187

REFERENCE 3: 77:101990

L21 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 13885-34-2 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-(1-cyclohexen-1-yloxy)-, (17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-3-ol, 17β-(1-cyclohexen-1-yloxy)- (8CI)
FS STEREOSEARCH
MF C24 H32 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation)
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 78:106316

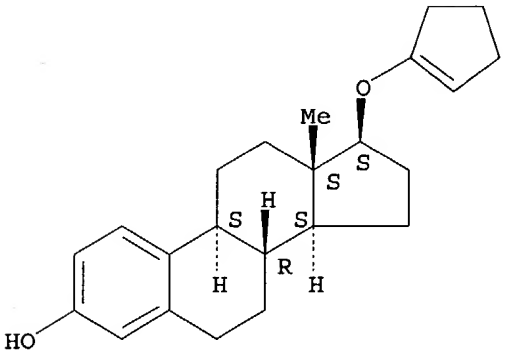
REFERENCE 2: 70:68634

REFERENCE 3: 66:95293

L21 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 13885-30-8 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17β-(1-cyclopenten-1-yloxy)- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H30 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB
(*File contains numerically searchable property data)
DT.CA CAplus document type: Patent

RL.P Roles from patents: PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

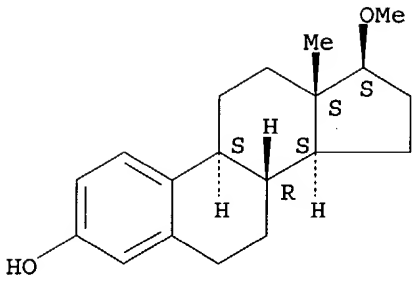
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 70:68634

REFERENCE 2: 66:95293

L21 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2004 ACS on STN
RN 4954-12-5 REGISTRY
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-3-ol, 17β-methoxy- (7CI, 8CI)
OTHER NAMES:
CN 17-Methoxy-1,3,5(10)-estratrien-3-ol
CN 17β-Methoxyestra-1,3,5(10)-trien-3-ol
FS STEREOSEARCH
MF C19 H26 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation); PRP (Properties)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

20 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
20 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 138:348841

REFERENCE 2: 136:85991

REFERENCE 3: 134:101056

REFERENCE 4: 130:293190

REFERENCE 5: 129:54482

REFERENCE 6: 116:235946

REFERENCE 7: 100:96847

REFERENCE 8: 89:2201

REFERENCE 9: 86:90134

REFERENCE 10: 82:125520

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(FILE 'REGISTRY' ENTERED AT 11:27:37 ON 20 JUL 2004)

FILE 'USPATFULL, USPAT2' ENTERED AT 11:29:09 ON 20 JUL 2004

FILE 'HCAPLUS' ENTERED AT 11:29:20 ON 20 JUL 2004

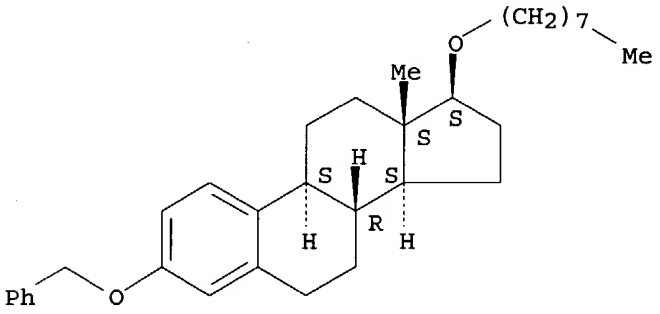
FILE 'REGISTRY' ENTERED AT 11:31:00 ON 20 JUL 2004
L61 10 S L5 NOT L21

=> d ide can tot

L61 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **319427-02-6** REGISTRY
CN Estra-1,3,5(10)-triene, 17-(octyloxy)-3-(phenylmethoxy)-, (17β)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H46 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

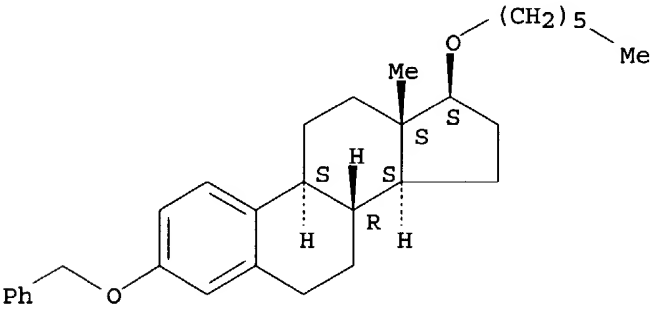
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **319427-01-5** REGISTRY
CN Estra-1,3,5(10)-triene, 17-(hexyloxy)-3-(phenylmethoxy)-, (17β)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H42 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

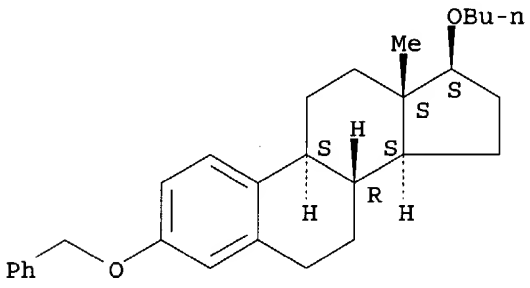
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **319427-00-4** REGISTRY
CN Estra-1,3,5(10)-triene, 17-butoxy-3-(phenylmethoxy)-, (17β)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C29 H38 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

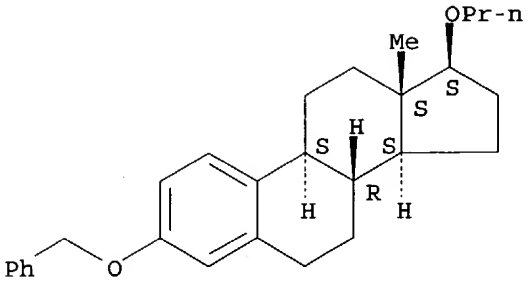
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **319426-99-8** REGISTRY
CN Estra-1,3,5(10)-triene, 3-(phenylmethoxy)-17-propoxy-, (17β)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C28 H36 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

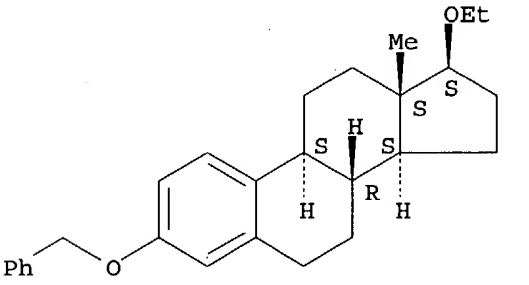
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **319426-98-7** REGISTRY
CN Estra-1,3,5(10)-triene, 17-ethoxy-3-(phenylmethoxy)-, (17β)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C27 H34 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

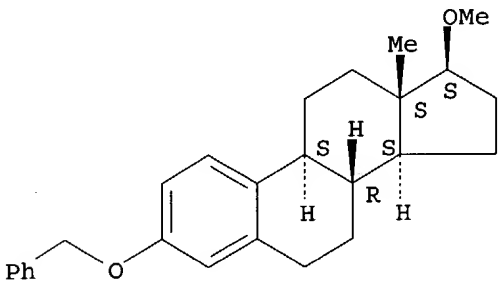
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

L61 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **141318-37-8** REGISTRY
CN Estra-1,3,5(10)-triene, 17-methoxy-3-(phenylmethoxy)-, (17β)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH
MF C26 H32 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

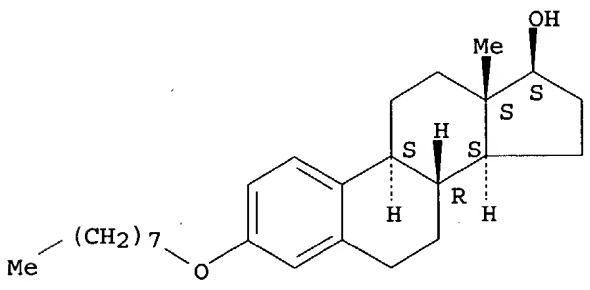
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 116:235946

L61 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **128805-68-5** REGISTRY
CN Estra-1,3,5(10)-trien-17-ol, 3-(octyloxy)-, (17β)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H40 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

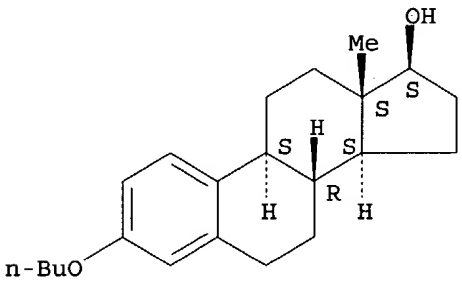
REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 114:218696

L61 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **21830-24-0** REGISTRY
CN Estra-1,3,5(10)-trien-17-ol, 3-butoxy-, (17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-17β-ol, 3-butoxy- (8CI)
FS STEREOSEARCH
MF C22 H32 O2
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:85991

REFERENCE 2: 134:101056

REFERENCE 3: 122:282544

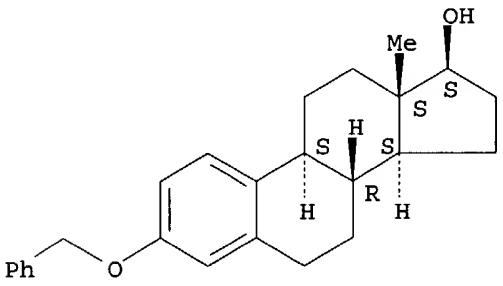
REFERENCE 4: 71:19218

REFERENCE 5: 70:97043

L61 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **14982-15-1** REGISTRY
CN Estra-1,3,5(10)-trien-17-ol, 3-(phenylmethoxy)-, (17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estra-1,3,5(10)-trien-17β-ol, 3-(benzyloxy)- (7CI, 8CI)
OTHER NAMES:
CN 3-(Benzyloxy)estra-1,3,5(10)-trien-17β-ol
CN 3-O-Benzylestradiol
CN BLE 99051

CN Estradiol 3-benzyl ether
FS STEREOSEARCH
MF C25 H30 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); PROC (Process); RACT (Reactant or reagent); NORL (No role in record)
RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

36 REFERENCES IN FILE CA (1907 TO DATE)
36 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 136:216934

REFERENCE 2: 136:85991

REFERENCE 3: 135:77015

REFERENCE 4: 134:326652

REFERENCE 5: 134:101056

REFERENCE 6: 131:88083

REFERENCE 7: 128:115126

REFERENCE 8: 124:270254

REFERENCE 9: 122:56574

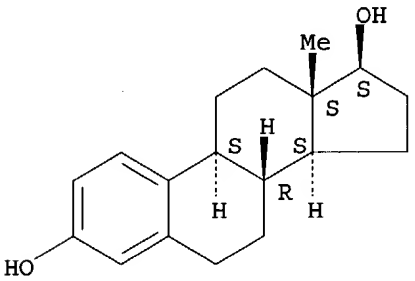
REFERENCE 10: 120:253366

L61 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2004 ACS on STN
RN **50-28-2** REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol (17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Estradiol (8CI)
OTHER NAMES:
CN (+)-3,17β-Estradiol
CN β-Estradiol

CN 13β-Methyl-1,3,5(10)-gonatriene-3,17β-ol
CN 17β-Estradiol
CN 17β-Oestradiol
CN 3,17-Epidihydroxyestratriene
CN 3,17β-Dihydroxyestra-1,3,5(10)-triene
CN 3,17β-Estradiol
CN Aerodiol
CN Altrad
CN Aquadiol
CN Bardiol
CN Beta-estradiol
CN Climaderm
CN Climara
CN Compudose
CN Compudose 200
CN Compudose 365
CN Corpagen
CN Dermestril
CN Dihydrofollicular hormone
CN Dihydrofolliculin
CN Dihydromenformon
CN Dihydrotheelin
CN Dihydroxyestrin
CN Dimenformon
CN Diogyn
CN Diogynets
CN Divigel
CN E 2
CN Encore
CN Epiestriol 50
CN Estra-1,3,5(10)-triene-3,17-diol, (17β)-
CN Estra-1,3,5(10)-triene-3,17β-diol
CN Estrace
CN Estraderm
CN Estraderm TTS
CN Estraderm TTS 100
CN Estraderm TTS 50
CN Estradot
CN Estraldine
CN Estring Vaginal Ring
CN Estroclim
CN Estroclim 50
CN Estrogel
CN Estrovite
CN Evorel
CN Femanest
CN Femestral
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use FCN, FIDE, or ALL for DISPLAY
FS STEREOSEARCH
MF C18 H24 O2
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IMSDRUGNEWS, IMSRESEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PHAR, PIRA, PROMT, PROUSDDR, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

52413 REFERENCES IN FILE CA (1907 TO DATE)
871 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
52493 REFERENCES IN FILE CAPLUS (1907 TO DATE)
12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 141:53559

REFERENCE 2: 141:53482

REFERENCE 3: 141:53474

REFERENCE 4: 141:52760

REFERENCE 5: 141:52323

REFERENCE 6: 141:52267

REFERENCE 7: 141:52248

REFERENCE 8: 141:52220

REFERENCE 9: 141:52046

REFERENCE 10: 141:51817

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FILE 'HCAOLD' ENTERED AT 11:32:29 ON 20 JUL 2004

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

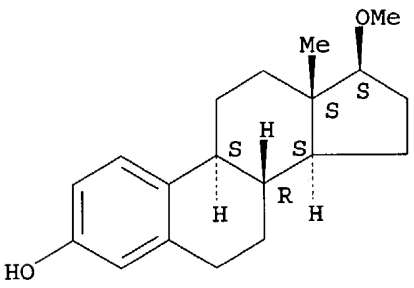
This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d all hitstr tot

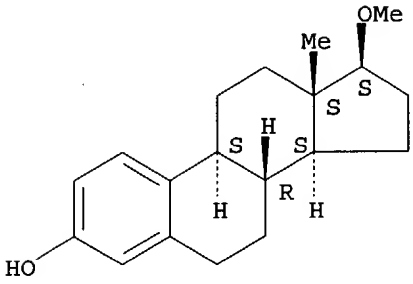
L62 ANSWER 1 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN
AN CA64:8257g CAOLD
TI 17β-estradiol 17-methyl ether
AU Coombs, M. M.; Roderick, H. R.
TI orientation of the fragmentation in mass spectrometry by the introduction of functional groups - (VII) ethylene ketals of 2-oxosteroids
AU Audier, Henri; Fetizon, M.; Gramain, J. C.
IT 700-77-6 1743-60-8 4832-17-1 4953-96-2 **4954-12-5**
4954-13-6 4954-14-7 4954-16-9 4954-17-0 4967-93-5 4967-94-6
4967-96-8 4967-97-9 4968-11-0 4999-72-8 5380-79-0 5506-56-9
6857-86-9
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



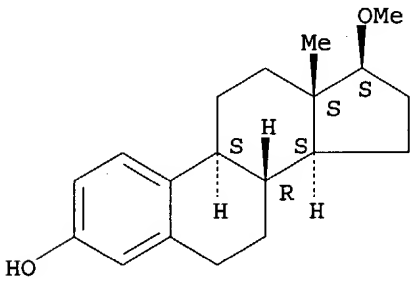
L62 ANSWER 2 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN
AN CA61:16379g CAOLD
TI fractionation of estrogen methyl esters with Al2O3 column chromatography-estimation of of 16-epiestriol in pregnancy urine
AU Shida, Keizo; Kimura, N.; Kambegawa, A.
IT 1474-53-9 3434-79-5 **4954-12-5**
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L62 ANSWER 3 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN
AN CA56:7630a CAOLD
TI steroid derivs. - (XII) chromatography of neutral steroids on a thin Al2O3 layer
AU Hermanek, Stanislav; Schwarz, V.; Cekan, Z.
IT 113-38-2 604-32-0 633-34-1 809-51-8 1061-54-7 1169-49-9
1175-12-8 1182-65-6 1235-98-9 1255-57-8 1259-22-9 1639-43-6
1639-44-7 1807-15-4 2080-86-6 2088-71-3 2099-26-5 3604-60-2
4139-90-6 4651-48-3 4860-15-5 **4954-12-5** 6252-45-5
14072-39-0 14546-23-7 19637-35-5 20272-84-8 20867-15-6 23838-12-2
29163-23-3 29789-88-6 31823-53-7 33854-98-7 34209-81-9 41329-03-7
50303-03-2 71205-59-9 82979-88-2 95557-72-5 95908-73-9 96273-79-9
96275-23-9 96345-96-9 96391-62-7 96553-92-3 96772-72-4 107158-49-6
IT **4954-12-5**
RN 4954-12-5 HCAOLD
CN Estra-1,3,5(10)-trien-3-ol, 17-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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